1 2 3 4 5 6 7 8 9
ring/chain nodes :
13 16 17
chain bonds :
7-11 8-10 11-12 12-13
ring/chain bonds :
13-16 13-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-9 7-8 8-9
exact/norm bonds :
5-7 6-9 7-8 8-9 13-16 13-17
exact bonds :
7-11 8-10 11-12 12-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom 16:CLASS 17:CLASS

Claim 32

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

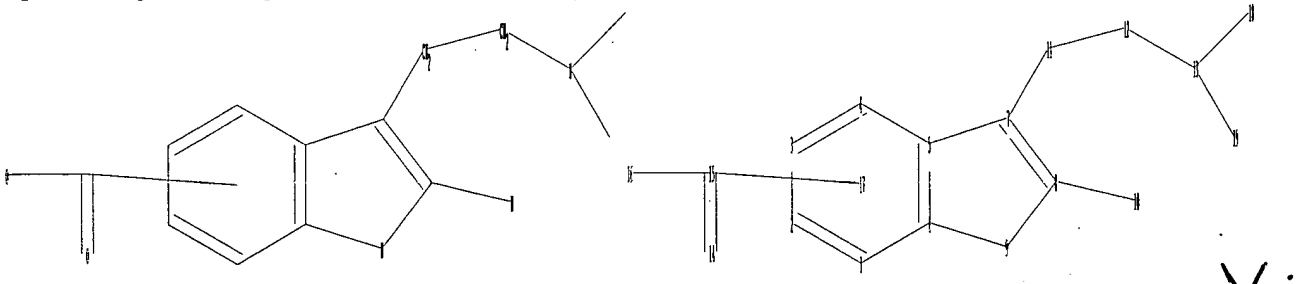
Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
FULL SEARCH INITIATED 15:56:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 325244 TO ITERATE

100.0% PROCESSED 325244 ITERATIONS 10 ANSWERS
SEARCH TIME: 00.00.02

L2 10 SEA SSS FUL L1

=>
Uploading C:\Program Files\Stnexp\Queries\10539151\claim 32 XIV5.str



chain nodes :
10 11 12 14 15 16
ring nodes :

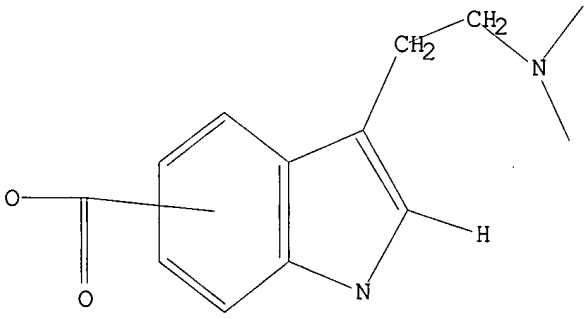
```
1  2  3  4  5  6  7  8  9
ring/chain nodes :
13  18  19
chain bonds :
7-11  8-10  11-12  12-13  14-15  15-16
ring/chain bonds :
13-18  13-19
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9
exact/norm bonds :
5-7  6-9  7-8  8-9  13-18  13-19  14-15  15-16
exact bonds :
7-11  8-10  11-12  12-13
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6


Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:Atom  18:CLASS
19:CLASS



L3      STRUCTURE UPLOADED

=> d
L3 HAS NO ANSWERS
L3                STR
```



XIV

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Structure attributes must be viewed using STN Express query preparation.


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FULL SEARCH INITIATED 15:56:49 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   325244 TO ITERATE

100.0% PROCESSED    325244 ITERATIONS                        15 ANSWERS
SEARCH TIME: 00.00.02

L4            15 SEA SSS FUL L3

=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              344.20     344.41
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FILE 'CAPLUS' ENTERED AT 15:56:56 ON 20 FEB 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 20 Feb 2007 VOL 146 ISS 9
FILE LAST UPDATED: 19 Feb 2007 (20070219/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

```
=> s l2
L5              8 L2

=> s l4
L6              9 L4

=> s l5 or l6
L7             17 L5 OR L6

=> d ibib abs hitstr L5 1-8
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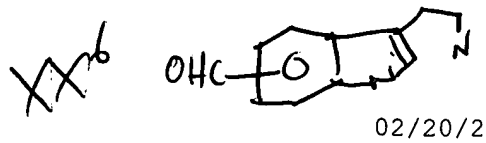


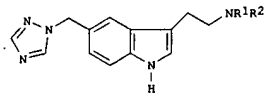
L5 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2005:811739 CAPLUS
DOCUMENT NUMBER: 143:229863
TITLE: A manufacturing of (triazolylmethyl)indole derivatives and their intermediates
INVENTOR(S): Martin, Pierre; Berens, Ulrich; Boudier, Andreas; Dosenbach, Oliver
PATENT ASSIGNEE(S): Ratiopharm G.m.b.H., Germany
SOURCE: PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005075422	A1	20050818	WO 2005-EP793	20050127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2553652	A1	20050818	CA 2005-2553652	20050127
EP 1751104	A1	20070214	EP 2005-707035	20050127
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				

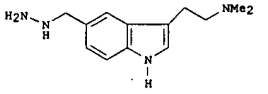
PRIORITY APPLN. INFO.: EP 2004-100303 A 20040128
US 2004-543463P P 20040210
WO 2005-EP793 W 20050127

OTHER SOURCE(S): MARPAT 143:229863
GI

L5 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

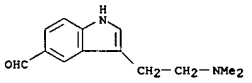


I



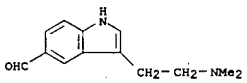
II

AB The invention relates to a preparation of (triazolylmethyl)indole derivs. of formula I [wherein: R1 and R2 are independently H or alkyl] and their intermediates. For instance, anti-migraine agent rizatriptan I [R1 = R2 = Me; no biol. data] was prepared from [(hydrazinomethylindolyl)ethyl]-dimethyl-amine II with a yield of 55%.
IT 152673-51-3P 862703-18-2P 862703-19-3P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(manufacturing of (triazolylmethyl)indole derivs. and their intermediates)
RN 152673-51-3 CAPLUS
CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 862703-18-2 CAPLUS
CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)

L5 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

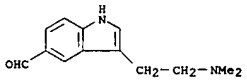


● HCl

RN 862703-19-3 CAPLUS
CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 152673-51-3
CMF C13 H16 N2 O



CM 2

CRN 144-62-7
CMF C2 H2 O4

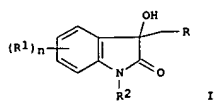
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:546477 CAPLUS
DOCUMENT NUMBER: 141:89009
TITLE: Synthesis of tryptamine derivatives and intermediates thereof
INVENTOR(S): Berens, Ulrich; Dosenbach, Oliver; Sprenger, Daniel
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056769	A2	20040708	WO 2003-EP50992	20031212
WO 2004056769	A3	20040916		
WO 2004056769	B1	20041104		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2508290	A1	20040708	CA 2003-2508290	20031212
AU 2003299227	A1	20040714	AU 2003-299227	20031212
EP 1572647	A2	20050914	EP 2003-780660	20031212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1729174	A	20060201	CN 2003-80107086	20031212
JP 2006516128	T	20060622	JP 2004-561492	20031212
US 2006058367	A1	20060316	US 2005-539151	20050616

PRIORITY APPLN. INFO.: EP 2002-406128 A 20021220
WO 2003-EP50992 W 20031212

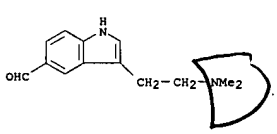
OTHER SOURCE(S): MARPAT 141:89009
GI



I

AB Indoleacetates I [R = CO2R3; R1 = (un)substituted alkyl, aryl, heterocyclyl, alkylsulfonyl, OH, SH, NO2, halogen, CN, CONH2, CONHNH2,

L5 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CO2H, alkenyl, alkynyl, cycloalkyl, acyloxy, NH2, NHNH2, B(OH)2; R2 = H, (un)substituted alkyl, CO2H, arylsulfonyl, alkylsulfonyl, aryl, CONH2, silyl; R3 = (un)substituted alkyl; n = 0-4] were prepd. and converted to I
[R = CONR4R5; R4, R5 = (un)substituted alkyl; R4R5 = (un)substituted alkylene] which were in turn converted to indoleacetamides and tryptamines. The synthesis methods and products are useful in the synthesis of pharmaceuticals. Thus, 5-bromoisatin was treated with CH2(CO2H)2 and ClCONMe2 to give I [R = CONMe2, R1 = 5-Br, R2 = H] which was treated with BF3.Et2O and BH3.Me2SO to give 2-(5-bromo-1H-indol-3-yl)-N,N-dimethylacetamide or with BF3.Et2O and NaBH4 to give [2-(5-bromo-1H-indol-3-yl)ethyl]-N,N-dimethylacetamide.
IT 152673-51-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tryptamine derivs. and intermediates thereof)
RN 152673-51-3 CAPLUS
CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

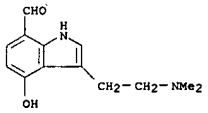


not claimed

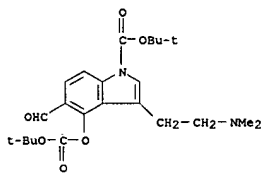
$R^3 + R^4$

cannot both be Me

L5 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 404887-83-8 CAPLUS
CN 1H-Indole-7-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-4-hydroxy- (9CI) (CA INDEX NAME)

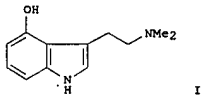


IT 404887-84-9P 404887-85-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of psilocin analogs having either a formyl group or bromine atom at the 5- or 7-position)
RN 404887-84-9 CAPLUS
CN 1H-Indole-1-carboxylic acid, 3-[2-(dimethylamino)ethyl]-4-[[(1,1-dimethylethoxy)carbonyl]oxy]-5-formyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



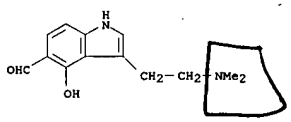
RN 404887-85-0 CAPLUS
CN 1H-Indole-1-carboxylic acid, 3-[2-(dimethylamino)ethyl]-4-[[(1,1-dimethylethoxy)carbonyl]oxy]-7-formyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L5 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:19828 CAPLUS
DOCUMENT NUMBER: 136:263284
TITLE: The chemistry of indoles. Part 109. Synthetic studies of psilocin analogs having either a formyl group or bromine atom at the 5- or 7-position
AUTHOR(S): Yamada, Fumio; Tamura, Mayumi; Hasegawa, Atsuko; Somei, Masanori
CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Kanazawa University, Kanazawa, 920-0934, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (2002), 50(1), 92-99
CODEN: CPBTAL; ISSN: 0009-2363
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:263284
GI

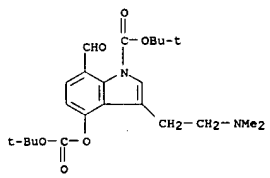


I

AB Psilocin (I) analogs having either a formyl group or a bromine atom at the 5- or 7-position have been prepared for the first time. Syntheses of 5- and 7-bromo derivs. of 4-hydroxy- and 4-benzyloxyindole-3-carbaldehyde, 4-benzyloxyindole-3-acetonitriles, and 4-benzyloxy-N,N-dimethyltryptamine have also been established.
IT 404887-81-6P 404887-83-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of psilocin analogs having either a formyl group or bromine atom at the 5- or 7-position)
RN 404887-81-6 CAPLUS
CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]-4-hydroxy- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:152309 CAPLUS
DOCUMENT NUMBER: 134:193415
TITLE: Preparation of heteroannelated pyridines as 5-HT1A receptor ligands
INVENTOR(S): Peglion, Jean-louis; Dessinges, Aimee; Poitevin, Christophe; Millan, Mark; Dekeyne, Anne
PATENT ASSIGNEE(S): Adir Et Compagnie, Fr.; Les Laboratoires Servier
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

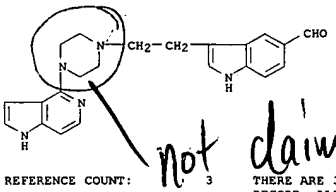
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1078928	A1	20010228	EP 2000-402359	20000825
EP 1078928	B1	20040512		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2797874	A1	20010302	FR 1999-10834	19990827
FR 2797874	B1	20020329		
US 6399616	B1	20020604	US 2000-641777	20000818
JP 2001097978	A	20010410	JP 2000-252191	20000823
JP 3602780	B2	20041215		
CA 2317053	A1	20010227	CA 2000-2317053	20000825
ZA 2000004411	A	20010228	ZA 2000-4411	20000825
CN 1286255	A	20010307	CN 2000-124065	20000825
HU 200003413	A2	20010730	HU 2000-3413	20000825
AT 266664	T	20040515	AT 2000-402359	20000825
PT 1078928	T	20040930	PT 2000-402359	20000825
ES 2220359	T3	20041216	ES 2000-402359	20000825
NO 2000004295	A	20010228	NO 2000-4295	20000828
NO 316651	B1	20040322		
BR 2000003848	A	20010403	BR 2000-3848	20000828
AU 765661	B2	20030925	AU 2000-53642	20000828
HK 1034250	A1	20050429	HK 2001-104815	20010711
US 2002161228	A1	20021031	US 2002-105171	20020325
US 6486171	B2	20021126		

PRIORITY APPLN. INFO.:
FR 1999-10834 A 19990827
US 2000-641777 A3 20000818

OTHER SOURCE(S): MARPAT 134:193415
GI

I

AB Title compds. [I; R1 = R(CH2)nZZ1; R = (un)substituted naphthyl or heteroannelated Ph; R2R3 = atoms to complete a thiophene, furan, or (oxo)pyrrole ring; Z = bons, O, [(ar)alkyl]imino; Z1 = 1,4-cyclohexylene, piperidine-1,4- or -4,1-diyl, piperazine-1,4-diyl; n = 1-6] were prepared Thus, 7-chlorofuro[2,3-c]pyridine was aminated by N-(2-naphthylmethyl)-4-piperidineamine to give I (R1 = RCH2NHZ1, R = 2-naphthyl, R2R3 = OCH:CH, Z1 = piperidine-4,1-diyl). Data for biol. activity of I were given.
IT 327173-90-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of heteroannelated pyridines as 5-HT1A receptor ligands)
RN 327173-90-0 CAPLUS
CN 1H-Indole-5-carboxaldehyde, 3-[2-[4-(1H-pyrrolo[3,2-c]pyridin-4-yl)-1-piperazinyl]ethyl]- (9CI) (CA INDEX NAME)



not claimed

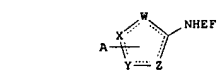
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:245114 CAPLUS
DOCUMENT NUMBER: 120:245114
TITLE: Preparation of heteroaromatic 5-hydroxytryptamine receptor agonists
INVENTOR(S): Castro Pineiro, Jose Luis; Matassa, Victor Giulio
PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9321182	A1	19931028	WO 1993-GB789	19930414
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9340766	A	19931118	AU 1993-40766	19930414
EP 636131	A1	19950201	EP 1993-910152	19930414
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07505649	T	19950622	JP 1993-518132	19930414
US 5510359	A	19960423	US 1994-318610	19941007

PRIORITY APPLN. INFO.:
GB 1992-8463 A 19920416
WO 1993-GB789 A 19930414

OTHER SOURCE(S): MARPAT 120:245114
GI



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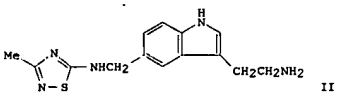
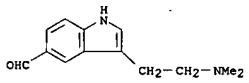


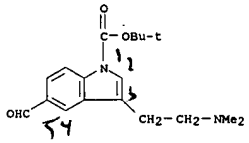
II

AB Title compds. I (W, X, Y, Z = O, S, N, C such that one of W, X, Y, Z = O, S and at least one of W, X, Y, Z = C; A = H, hydrocarbyl, heterocyclyl, halo, NC, F3C, RxO, RxS, RyRxN, RyCORxN, RyO2CRxN, etc. wherein Rx, Ry = H, hydrocarbyl, heterocyclyl, RxRy = C2-6 alkylene; E = bond, C13-4 alkylene; F = substituted heterocyclyl) or a salt thereof, are prepared
To
5-(aminomethyl)-3-[2-(N-tert-butoxycarbonylamino)ethyl]-14-indole (preparation
given) in THF and (Me2CH)2NEt was added 5-chloro-3-methyl-1,2,4-thiadiazole to give the protected thiadiazolylamine which in CH2Cl2 was reacted with F3CCO2H to give the title compound II. The activity of I as agonists of 5-HT1 receptors was measured as to their ability to mediate contraction of the saphencus vein and calculated as -log10EC50(pEC50)
from

L5 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
plots of % 5-HT (1 μM) response against the concn. of the agonist and was not less than 5.0. A tablet formulation comprising I is given.
IT 152673-51-3P 152673-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of 5-HT1 agonists)
RN 152673-51-3 CAPLUS
CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 152673-52-4 CAPLUS
CN 1H-Indole-1-carboxylic acid, 3-[2-(dimethylamino)ethyl]-5-formyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:107034 CAPLUS
DOCUMENT NUMBER: 120:107034
TITLE: Imidazole, triazole and tetrazole serotonin 5-HT1 receptor antagonists
INVENTOR(S): Castro, Pineiro Jose Luis; Matassa, Victor Giulio
PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9320066	A1	19931014	WO 1993-GB652	19930329
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9338956	A	19931108	AU 1993-38956	19930329
AU 675641	B2	19970213		
EP 637307	A1	19950208	EP 1993-907945	19930329
EP 637307	B1	20001108		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07505382	T	19950615	JP 1993-517223	19930329
JP 3285581	B2	20020527		
AT 197453	T	20001111	AT 1993-907945	19930329
ES 2152948	T3	20010216	ES 1993-907945	19930329
US 5607957	A	19970304	US 1994-313058	19940929

PRIORITY APPLN. INFO.: GB 1992-7396 A 19920403
WO 1993-GB652 A 19930329

OTHER SOURCE(S): MARPAT 120:107034
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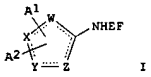
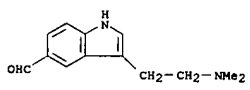


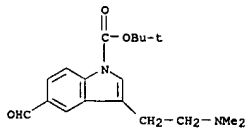
I

AB The title compds. I [A1, A2 = H, hydrocarbon group, heterocyclic group, halogen, CN, CF3, (un)substituted amino, etc.; E = direct bond, (un)branched C1-4 alkylene; F = (un)substituted heterocyclyl; 2-4 of W, X, Y, and Z = N and the remainder are C; when W = X = Y = Z = N then A2 = nonbonded electron pair], which are serotonin 5-HT1 receptor antagonists (no data) and useful in the treatment of migraine headache (no data), are prepared and I-containing formulations presented. Thus, 3-[2-(dimethylamino)ethyl]-5-[(2-methyl-1,2,4-triazol-3-yl)aminomethyl]-1H-indole oxalate (m.p. 208-210°) was prepared from 2-methyl-3-nitro-1,2,4-triazole in 3 steps.

L5 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 152673-51-3P 152673-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of serotonin 5-HT1 receptor antagonists)
RN 152673-51-3 CAPLUS
CN 1H-Indole-5-carboxaldehyde, 3-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 152673-52-4 CAPLUS
CN 1H-Indole-1-carboxylic acid, 3-[2-(dimethylamino)ethyl]-5-formyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

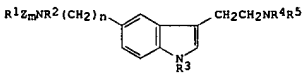


L5 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1987:575786 CAPLUS
DOCUMENT NUMBER: 107:175786
TITLE: Preparation of 5-(2-aminoethyl)tryptamines as antimigraine agents
INVENTOR(S): Mills, Keith; Coates, Ian Harold; Bays, David Edmund; Webb, Colin Frederick; Dowle, Michael Dennis
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Ger. Offen., 17 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3700407	A1	19870709	DE 1987-3700407	19870108
AU 8767418	A	19870709	AU 1987-67418	19870108
AU 597324	B2	19900531		
NL 8700027	A	19870803	NL 1987-27	19870108
GB 2186874	A	19870826	GB 1987-381	19870108
GB 2186874	B	19900207		
FR 2595352	A1	19870911	FR 1987-108	19870108
FR 2595352	B1	19900713		
JP 62228057	A	19871006	JP 1987-2590	19870108
AT 8700024	A	19871215	AT 1987-24	19870108
AT 386197	B	19880711		
ZA 8700104	A	19871230	ZA 1987-104	19870108
BE 1000072	A1	19880202	BE 1987-4	19870108
CH 671017	A5	19890731	CH 1987-46	19870108

PRIORITY APPLN. INFO.: GB 1986-398 A 19860108

OTHER SOURCE(S): MARPAT 107:175786
GI



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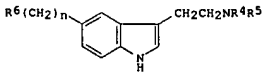
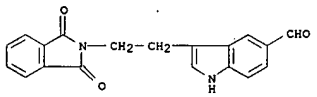
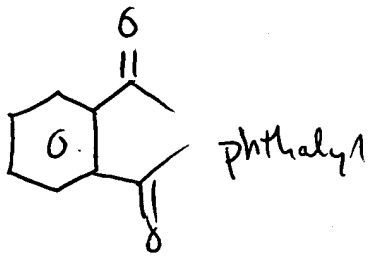


II

AB The title compds. (I; R1 = H, C1-6 alkyl, C3-7 cycloalkyl, Ph, phenyl-C1-4 alkyl; R2, R3 = H, C1-3 alkyl; R4, R5 = CH2CH:CH2, R3; Z = CO, SO2; n = 2-5; m = 1) were prepared as antimigraine agents (no data). 4-H2NNHC6H4CH2CN was refluxed with 4-phthalimidobutanal di-Et acetal in H2O/HOAc to give tryptamine II (NR4R5 = phthalimido, R6 = cyano, n = 1) which, on hydrogenation over PdO/C, gave II.HCl (NR4R5 = phthalimido, R6

L5 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
NH2, n = 2). This was stirred with Ac2O in pyridine and the product refluxed with H2NNH2 in EtOH to give II (R4 = R5 = H, R6 = AcNH, n = 2). Tablets were prepd. each contg. II (R4 = R5 = Me, R6 = 4-AcNHC6H4CH2CONH, n = 2) 2.4, CaHPO4 95.1, Croscarmellose Na 2.0, and Mg stearate 0.5 mg.
IT 105323-64-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reaction of)
RN 105323-64-6 CAPLUS
CN 1H-Indole-5-carboxaldehyde, 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]- (9CI) (CA INDEX NAME)



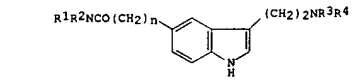


L5 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1986:626347 CAPLUS
DOCUMENT NUMBER: 105:226347
TITLE: Indole derivatives and pharmaceutical compositions containing them
INVENTOR(S): Bays, David Edmund; Webb, Colin Frederick
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Ger. Offen., 60 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3543982	A1	19860619	DE 1985-3543982	19851212
BE 903846	A1	19860612	BE 1985-216004	19851212
SE 8505887	A	19860614	SE 1985-5887	19851212
GB 2168347	A	19860618	GB 1985-30591	19851212
GB 2168347	B	19880203		
AU 8551151	A	19860619	AU 1985-51151	19851212
AU 579687	B2	19881201		
FR 2574793	A1	19860620	FR 1985-18416	19851212
FR 2574793	B1	19881014		
NL 8503424	A	19860701	NL 1985-3424	19851212
JP 61151172	A	19860709	JP 1985-278124	19851212
ZA 8509520	A	19860827	ZA 1985-9520	19851212
CH 667454	A5	19881014	CH 1985-5301	19851212

PRIORITY APPLN. INFO.: GB 1984-31426 A 19841213

OTHER SOURCE(S): CASREACT 105:226347; MARPAT 105:226347
GI



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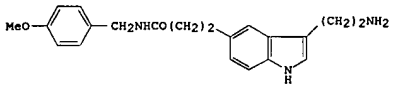
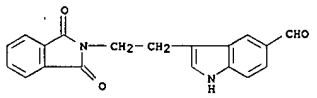


II

AB Indoles I [R1 = H, C1-6 alkyl, C3-7 cycloalkyl, C3-6 alkenyl, Ph or phenyl-C1-4-alkyl with Ph (un)substituted by C1-3 alkoxy, OH, halo, R5R6NCO (R5, R6 = H, C1-3 alkyl), R7R8N (R7, R8 = H, C1-3 alkyl; R7R8N = saturated monocyclic 5-7 membered ring); R2 = H, C1-6 alkyl; R1R2N = R7R8N;

L5 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
R3, R4 = H, C1-3 alkyl, 2-propenyl; n = 2-5] and their physiol. tolerable salts and solvates, useful as selective vasoconstrictors for cranial vessels at 0.5-50 mg, were prepd. by 7 methods. 4-H2NC6H4(CH2)2CO2H was diazotized and the product reduced with SnCl2 to give 4-H2NNHC6H4(CH2)2CO2H.HCl, which reacted with 2-(4,4-diethoxybutyl)-1H-isoindole-1,3(2H)-dione in refluxing aq. AcOH to give 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]-1H-indole-5-propanoic acid. Successive reaction with pivaloyl chloride and 4-MeOC6H4CH2NH2 gave the N-[(4-methoxyphenyl)methyl]propanamide analog, hydrazinolysis of which gave indolylethylamine II, characterized as the hemisuccinate. Formulations for tablets, capsules, suppositories, and i.v. injection solns. were given.
IT 105323-64-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Wittig reaction of)
RN 105323-64-6 CAPLUS
CN 1H-Indole-5-carboxaldehyde, 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]- (9CI) (CA INDEX NAME)



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L3             STRUCTURE UPLOADED
L4          15 S L3 FULL

     FILE 'CAPLUS' ENTERED AT 15:56:56 ON 20 FEB 2007
L5           8 S L2
L6           9 S L4
L7          17 S L5 OR L6

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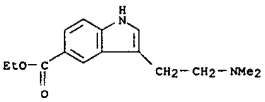
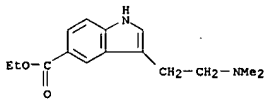
L6 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2003:234500 CAPLUS
DOCUMENT NUMBER: 139:52822
TITLE: Synthesis of [3-[2-(dimethylamino)ethyl]-2-[[3-(dimethylamino)ethyl]-1H-indol-5-yl] methyl]-1H-indol-5-yl]-N-methylmethanesulfonamide - the main sumatriptan impurity
AUTHOR(S): Skwierawska, A.; Paluszkiewicz, E.
CORPORATE SOURCE: Department of Chemistry, Gdansk University of Technology, Gdansk, 80-952, Pol.
SOURCE: Polish Journal of Chemistry (2003), 77(3), 329-332
CODEN: PJCHDQ; ISSN: 0137-5083
PUBLISHER: Polish Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:52822
AB Alkylation of sumatriptan in position 2 by 3-[2-(dimethylamino)ethyl]-5-indolemethanol is described. Alternative multistep synthesis of 3-[2-(dimethylamino)ethyl]-5-indolemethanol is presented.
IT 137499-21-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of [3-[2-(dimethylamino)ethyl]-2-[[3-(dimethylamino)ethyl]-1H-indol-5-yl] methyl]-1H-indol-5-yl]-N-methylmethanesulfonamide via Fischer indole synthesis)
RN 137499-21-9 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



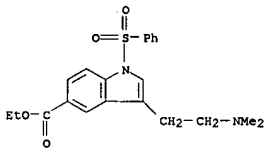
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L6 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L6 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:83714 CAPLUS
DOCUMENT NUMBER: 134:311061
TITLE: Synthesis of 5-(sulfamoylmethyl)indoles
AUTHOR(S): Bosch, J.; Roca, T.; Armengol, M.; Fernandez-Forner, D.
CORPORATE SOURCE: Laboratory of Organic Chemistry, Faculty of Pharmacy, University of Barcelona, Barcelona, 08028, Spain
SOURCE: Tetrahedron (2001), 57(6), 1041-1048
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:311061
AB The synthesis of 5-(sulfamoylmethyl)indoles bearing a two-carbon chain at C-3 (aminoethyl, acetate, hydroxyethyl, ethyl) either by the Grandberg modification of the Fischer indolization or by intramol. Heck reaction of suitable o-halotrifluoroacetanilides is reported.
IT 137499-21-9P 334981-33-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 5-(sulfamoylmethyl)indoles)
RN 137499-21-9 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 334981-33-8 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-1-(phenylsulfonyl)-, ethyl ester (9CI) (CA INDEX NAME)

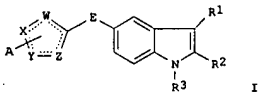


REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS

L6 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:610523 CAPLUS
DOCUMENT NUMBER: 123:9441
TITLE: Indole-substituted five-membered heteroaromatic compounds as 5-HT1 receptor agonists
INVENTOR(S): Baker, Raymond; Reeve, Austin J.; Street, Leslie J.
PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK
SOURCE: U.S., 31 pp. Cont. of U.S. Ser. No. 641,422, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5317103	A	19940531	US 1992-914683	19920716
PRIORITY APPLN. INFO.:			US 1991-641422	B1 19910115

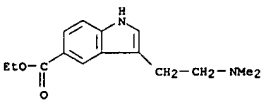
OTHER SOURCE(S): MARPAT 123:9441
GI



I

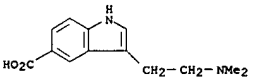
AB The title compds. [I; A = H, halogen, CN, NO2, CF3, (un)substituted NH2, etc.; E = (un)branched C1-4 alkylene, direct bond; R1 = (un)substituted aminoalkyl, (un)substituted heterocyclyl; R2, R3 = H, C1-6 alkyl, alkenyl, alkynyl; W, X, Y, Z = O, S, N, C; where >1 of W, X, Y, Z = O or S and >1 of W, X, Y, Z = C], useful as specific agonists of 5-HT1-like receptors (no data) and which are useful in the treatment of migraine headache and associated disorders (no data), are prepared and I-containing formulations presented. Thus, 2-[5-[5-(3-benzyl-1,2,4-oxadiazol)-yl]-1H-indol-3-yl]ethylamine hydrogen oxalate hydrate, m.p. 229°, was prepared
IT 137499-21-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of indole-substituted 5-membered heteroaroms. as 5-HT1 receptor agonists)
RN 137499-21-9 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester (9CI) (CA INDEX NAME)

L6 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



V

IT 114365-09-2P 163797-85-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indole-substituted 5-membered heteroaroms. as 5-HT1 receptor agonists)
RN 114365-09-2 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)

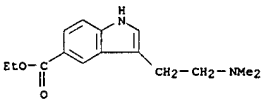


V

RN 163797-85-1 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester, ethanedioate (9CI) (CA INDEX NAME)

CM 1

CRN 137499-21-9
CMF C15 H20 N2 O2



V

CM 2

CRN 144-62-7
CMF C2 H2 O4

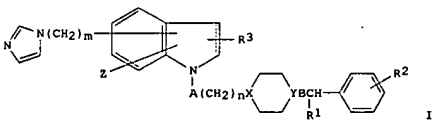
L6 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L6 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN

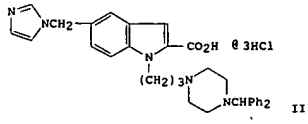
ACCESSION NUMBER: 1994:134530 CAPLUS
DOCUMENT NUMBER: 120:134530
TITLE: Preparation of (imidazolyl- and imidazolylalkyl)indole derivatives as inhibitors of thromboxane A2 synthesis and histamine
INVENTOR(S): Matsui, Hiroshi; Kamiya, Shoji; Shirahase, Hiroaki; Nakamura, Shohei
PATENT ASSIGNEE(S): Kyoto Pharmaceutical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 73 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9320065	A1	19931014	WO 1993-JP378	19930326
W: AU, CA, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2109931	A1	19931014	CA 1993-2109931	19930326
AU 9337680	A	19931108	AU 1993-37680	19930326
AU 658729	B2	19950427		
EP 597112	A1	19940518	EP 1993-906837	19930326
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
US 5538973	A	19960723	US 1995-393042	19950223
PRIORITY APPLN. INFO.:			JP 1992-102071 A	19920327
			WO 1993-JP378 A	19930326
			US 1993-142443 B1	19931126

OTHER SOURCE(S): MARPAT 120:134530
GI



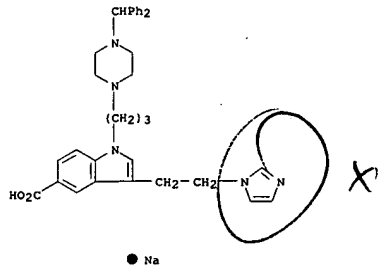
I



II

L6 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

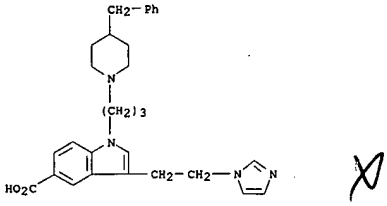
AB The title compds. (I; R1 = H, aryl; R2 = H, halo, lower alkyl or alkoxy; R3 = H, lower alkyl; A = bond, CO, CH2CO, CONH, COCH2O, alkyleneoxy; B = bond, O, alkylene, alkyleneoxy; X = Y = N or one of X and Y = N and the other = CH; Z = H, CO2H or its ester; m, n = 0-4), also having vasodilating and blood platelet aggregation-inhibiting activity and inhibiting histamine- and leukotriene-induced contraction of a respiratory tract and useful for prevention and/or treatment of diseases induced by thromboxane A2 or histamine, e.g. asthma and allergy, are prepared Thus, alkylation of 2-ethoxycarbonyl-5-(1H-imidazol-ylmethyl)-1H-indole by Br(CH2)3Cl in the presence of NaH in DMF and condensation of the resulting 1-(3-chloropropyl)indole derivative with 1-diphenylmethylpiperazine in the presence of K2CO3 and NaI in DMF at 80° gave, after saponification with NaOH in 95% aqueous EtOH and acidification with 3 N aqueous HCl, an (imidazolylpropyl)indoline derivative (II). II at 10-5 M in vitro inhibited 100% the histamine-induced contraction of guinea pig's lungs and at 30 mg/kg p.o. in vivo inhibited the histamine- and leukotriene D4-induced contraction of respiratory tract by 100 and 75%, resp.
IT 152631-38-4P 152631-39-5P 152631-40-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as thromboxane A synthesis and histamine inhibitor)
RN 152631-38-4 CAPLUS
CN 1H-Indole-5-carboxylic acid, 1-[3-[4-(diphenylmethyl)-1-piperazinyl]propyl]-3-[2-(1H-imidazol-1-yl)ethyl]-, sodium salt (9CI) (CA INDEX NAME)



● Na

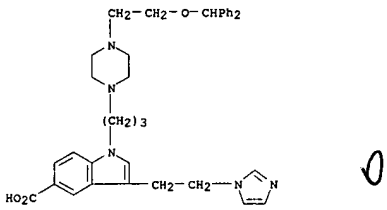
RN 152631-39-5 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(1H-imidazol-1-yl)ethyl]-1-[3-[4-(phenylmethyl)-1-piperidinyl]propyl]-, sodium salt (9CI) (CA INDEX NAME)

L6 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



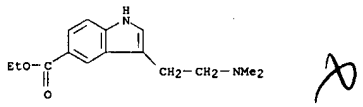
● Na

RN 152631-40-8 CAPLUS
CN 1H-Indole-5-carboxylic acid, 1-[3-[4-[2-(diphenylmethoxy)ethyl]-1-piperazinyl]propyl]-3-[2-(1H-imidazol-1-yl)ethyl]-, sodium salt (9CI) (CA INDEX NAME)

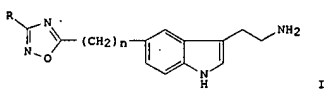


● Na

L6 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 137499-21-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of, with amide oximes, oxadiazoles from)
RN 137499-21-9 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:603336 CAPLUS
DOCUMENT NUMBER: 119:203336
TITLE: Synthesis and serotonergic activity of 5-(oxadiazolyl)tryptamines: potent agonists for 5-HT1D receptors
AUTHOR(S): Street, Leslie J.; Baker, Raymond; Castro, Jose L.; Chambers, Mark S.; Guiblin, Alexander R.; Hobbs, Sarah C.; Matassa, Victor G.; Reeve, Austin J.; Beer, Margaret S.; et al.
CORPORATE SOURCE: Chem. Dep., Merck Sharp and Dohme Res. Lab., Harlow/Essex, CM20 2QR, UK
SOURCE: Journal of Medicinal Chemistry (1993), 36(11), 1529-38
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

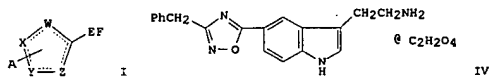


AB The synthesis and 5-HT1D receptor activity of a novel series of 5-(oxadiazolyl)tryptamines I (R = Me, Et, H2N, Ph, PhCH2, 4-MeSO2NHC6H4CH2, etc.; n = 0-3) is described. Modifications of the oxadiazole 3-substituent, length of the linking chain (n), and the amine substituents are explored and reveal a large binding pocket in the 5-HT1D receptor domain. Oxadiazole substituents such as benzyl are accommodated without loss of agonist potency or efficacy. The incorporation of polar functionality on a Ph or benzyl spacer group results in a 10-fold increase in affinity and functional potency. Optimal 5-HT1D activity is observed when the heterocycle is conjugated with the indole and the benzyl sulfonamides represent some of the most potent 5-HT1D agonists known. Replacement of O for S in the heterocycle leads to a further increase in potency. Deletion of oxadiazole N-2 does not reduce activity, suggesting the requirement for only one H-bond acceptor in this location. The selectivity of these compds. for 5-HT1D receptors over other serotonergic receptors is discussed. Sulfonamide I (R = 4-MeSO2NHC6H4CH2, n = 0) shows ≥1000-fold selectivity for 5-HT1D over 5-HT2, 5-HT1C, and 5-HT3 receptors and 10-fold selectivity with respect to 5-HT1A receptors. The functional activity of this series of compds. is studied and demonstrates high 5-HT1D receptor potency and efficacy comparable to that of 5-HT.

L6 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:83677 CAPLUS
DOCUMENT NUMBER: 116:83677
TITLE: Preparation of substituted (1,2,4-oxadiazolylindolyl)ethylamine and analogs as agonists of 5-HT1-like receptors
INVENTOR(S): Baker, Raymond; Reeve, Austin J.; Street, Leslie J.
PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK
SOURCE: Eur. Pat. Appl., 58 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

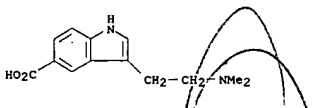
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 438230	A2	19910724	EP 1991-300180		19910110
EP 438230	A3	19920212			
EP 438230	B1	19970423			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE					
AT 152110	T	19970515	AT 1991-300180		19910110
CA 2034189	A1	19910718	CA 1991-2034189		19910115
FI 9100228	A	19910718	FI 1991-228		19910116
NO 9100187	A	19910718	NO 1991-187		19910116
AU 9169440	A	19910725	AU 1991-69440		19910116
CN 1053429	A	19910731	CN 1991-100380		19910117
JP 06100558	A	19940412	JP 1991-216736		19910117
PRIORITY APPLN. INFO.:			GB 1990-1018	A	19900117
			GB 1990-8587	A	19900417

OTHER SOURCE(S): MARPAT 116:83677
GI

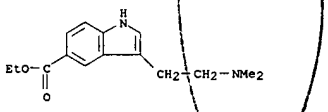


AB Title compds. I [wherein the broken circle represents 2 non-adjacent double bonds in any position; W, X, Y, Z = O, S, N, C, such that 1 of W, X, Y, Z = O, S and at least 1 of W, X, Y, Z = C; A = H, hydrocarbyl, halo, NC, F3C, O2N, etc.; E = bond, C1-4 alkylene, F = (substituted) heterocyclyl] or a salt or prodrug thereof, are prepared NaNO2 was added to 4-(H2N)C6H4CO2Et in concentrated HCl, the mixture stirred at 0° before adding SnCl2.2H2O in HCl to give 4-(H2NNH)C6H4CO2Et.HCl (II). II and 4-ClCH2(CH2)2CH(OMe)2 in EtOH/H2O were refluxed, the solvent removed and the residue chromatographed to give 2-(5-5-carbethoxy-1H-indol-3-yl)ethylamine.H maleate (III). NaH was added to phenylacetamide oxime in THF, the reaction mixture refluxed, III was added and the whole refluxed for 2 h, the reaction mixture cooled to room temperature to give the title compound as

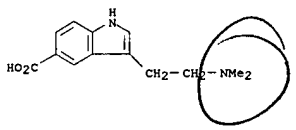
L6 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
the H.oxalate (IV). The activity as agonist of 5-HT1-like receptor was measured in terms of their ability to mediate contraction of the saphenous
vein of rabbits, and the potency calcd. as -log10EC50 (pEC50). The pEC50 of IV was not less than 5.0. Tablet compns. comprising I are given.
IT 114365-09-2P 137499-21-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of 5-HT1 agonists)
RN 114365-09-2 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



RN 137499-21-9 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, ethyl ester (9CI) (CA INDEX NAME)



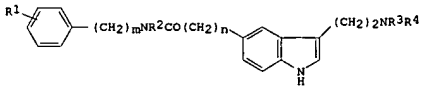
L6 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(II). Tablets for oral administration contained II 10, Mg stearate BP 0.5, and anhyd. lactose 99 mg per tablet.
IT 114365-09-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in synthesis of indole cranial vasoconstrictor)
RN 114365-09-2 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:204491 CAPLUS
DOCUMENT NUMBER: 108:204491
TITLE: Indole derivatives, procedure for their preparation, and their use as selective cranial vasoconstrictors for treating migraine or cluster headaches
INVENTOR(S): Oxford, Alexander William; Coates, Ian Harold; Bays, David Edmund; Webb, Colin Frederick
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Ger. Offen., 19 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3719699	A1	19871217	DE 1987-3719699	19870612
GB 2191488	A	19871216	GB 1987-13817	19870612
GB 2191488	B	19900328		
AU 8774188	A	19871217	AU 1987-74188	19870612
FR 2600061	A1	19871218	FR 1987-8193	19870612
FR 2600061	B1	19890707		
NL 8701372	A	19880104	NL 1987-1372	19870612
JP 63022068	A	19880129	JP 1987-146805	19870612
ZA 8704234	A	19880427	ZA 1987-4234	19870612
BE 1000338	A4	19881025	BE 1987-648	19870612
CH 673841	A5	19900412	CH 1987-2209	19870612
PRIORITY APPLN. INFO.:			GB 1986-14287 A	19860612

OTHER SOURCE(S): CASREACT 108:204491; MARPAT 108:204491
GI



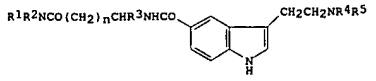
I

AB Indole derivs. I [R1 = NR5R6, (CH2)pCO2R5, (CH2)pCONR5R6, (CH2)pNHCOR5, (CH2)pO2SNR5R6, (CH2)pNHO2SR7; R5, R6 = H, alkyl; NR5R6 = monocyclic heterocyclyl; R7 = alkyl; p = 0, 1; R2 = H, alkyl; R3, R4 = H, alkyl, 2-propenyl; m = 0-4;f n = 0, 1; m and n may not both = 0] and their physiol. tolerable salts and solvates, selective vasoconstrictors for cranial blood vessels and thus useful against migraine and cluster headaches (no data), were prepared by 8 methods. 3-[2-[[(Phenylmethoxy)carbonyl]amino]ethyl]-1H-indole-5-carboxylic acid in THF was refluxed with 1,1'-carbonyldiimidazole, then treated with 4-Me2NC6H4CH2CH2NH2 to give I (R1 = 4-Me2N, R2 = R3 = H, R4 = CO2Ph, m = 2, n = 0) which was deblocked with H2 over 10% Pd/C to give I (R1 = 4-Me2N, R2 = R3 = R4 = H, m = 2, n = 0), characterized as the HCl salt

L6 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1988:150306 CAPLUS
DOCUMENT NUMBER: 108:150306
TITLE: Preparation and formulation of 1H-indole-5-carboxamide useful for treatment of migraine
INVENTOR(S): Oxford, Alexander William; Dowle, Michael Dennis
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Eur. Pat. Appl., 21 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 244085	A2	19871104	EP 1987-302654	19870327
EP 244085	A3	19880420		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
AU 8770720	A	19871001	AU 1987-70720	19870327
AU 602888	B2	19901101		
JP 63017860	A	19880125	JP 1987-73946	19870327
ZA 8702263	A	19880330	ZA 1987-2263	19870327
US 4795756	A	19890103	US 1987-30625	19870327
PRIORITY APPLN. INFO.:			GB 1986-7824 A	19860327

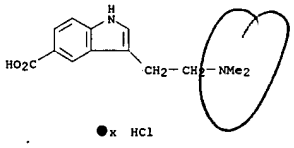
OTHER SOURCE(S): MARPAT 108:150306
GI



I

AB Title compds., I [R1 = H, C1-6 alkyl, C3-7 cycloalkyl, (un)substituted Ph; R2 = H, C1-6 alkyl; R3 = H, C1-3 alkyl; R4, R5 = H, C1-3 alkyl, H2C:CHCH2; n = 0, 1] and their salts, hydrates, useful for the treatment of migraine (no data), were prepared PhCH2 2-[5-[[[(diphenylamino)carbonyl]oxo]carbonyl]-1H-indol-3-yl]ethyl carbamate, H2NCH2CONH2·HCl, and NaOAc in DMF were reacted at room temperature to give the [[(aminooxoethyl)amino]carbonyl] derivative which was hydrogenated over PdO/C to give the indolecarboxamide derivative which with PhCHO in EtOH and NaBH4 was converted to the phenylmethylamino derivative, and to this was added Me2SO4 and K2CO3 in DMF to give the N-Me derivative, which in EtOH was hydrogenated over Pd/C to give I (R1-R4 = H; R5 = Me; n = 0). A tablet formulation comprised II 100, Mg stearate 1, and anhydrous lactose 99 mg/tablet.
IT 113438-61-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

L6 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(Reactant or reagent)
(prepn. and amidation of)
RN 113438-61-2 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(dimethylamino)ethyl]-, hydrochloride (9CI) (CA INDEX NAME)

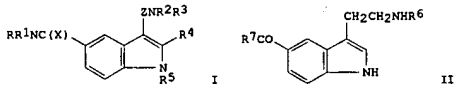


L6 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1980:532369 CAPLUS
DOCUMENT NUMBER: 93:132369
TITLE: Indole compounds and pharmaceutical compositions containing them
INVENTOR(S): Webb, Colin Frederick
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Ger. Offen., 102 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

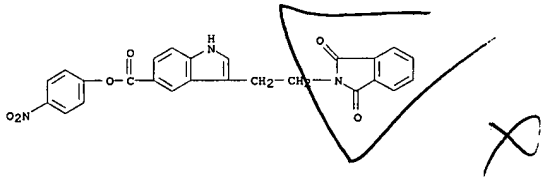
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2940687	A1	19800430	DE 1979-2940687	19791008
DE 2940687	C2	19910801		
ZA 7905239	A	19801126	ZA 1979-5239	19791002
FI 7903071	A	19800413	FI 1979-3071	19791004
DK 7904255	A	19800413	DK 1979-4255	19791009
AU 7951657	A	19800417	AU 1979-51657	19791010
AU 534705	B2	19830908		
GB 2035310	A	19800618	GB 1979-35208	19791010
GB 2035310	B	19821222		
US 4252803	A	19810224	US 1979-83343	19791010
AT 7906605	A	19840815	AT 1979-6605	19791010
AT 377511	B	19850325		
SE 7908443	A	19800413	SE 1979-8443	19791011
SE 448628	B	19870309		
SE 448628	C	19870618		
ES 484980	A1	19801101	ES 1979-484980	19791011
CH 646151	A5	19841115	CH 1979-9194	19791011
BE 879381	A1	19800201	BE 1979-197621	19791012
NL 7907583	A	19800415	NL 1979-7583	19791012
FR 2438651	A1	19800509	FR 1979-25446	19791012
FR 2438651	B1	19830304		
JP 55062063	A	19800510	JP 1979-130944	19791012
JP 63058817	B	19881117		
CA 1146550	A1	19830517	CA 1979-337443	19791012
ES 492114	A1	19810716	ES 1980-492114	19800603

PRIORITY APPLN. INFO.: GB 1978-40279 A 19781012

OTHER SOURCE(S): MARPAT 93:132369
GI



L6 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
AB The indole derivs. I [R, R1, R2, R3 = H, (substituted) alkyl, cycloalkyl, aryl, or aralkyl; RR1N, and R2R3N = ring; R4 = H, C1-3 alkyl, aryl; R5 = H, alkyl, aralkyl; Z = C1-4 alkylene; X = O, S] and their salts were prepared for use in treatment of hypertension and migraines (no data). Thus, II (R6 = CO2CH2Ph, R7 = OH) reacted with PhCH2NH2 in the presence of
2-chloro-1-methylpyridinium iodide to give II (R6 = CO2CH2Ph, R7 = NHCH2Ph), which was hydrogenated over Pd-C to give I (R6 = H, R7 = NHCH2Ph), isolated as compound with creatinine sulfate.
IT 74884-82-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and amidation of)
RN 74884-82-5 CAPLUS
CN 1H-Indole-5-carboxylic acid, 3-[2-(1,3-dihydro-1,3-dioxo-2H-isoindol-2-yl)ethyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)



STN

Reg/Caplus

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10  11  13  16  17
ring nodes :
1  2  3  4  5  6  7  8  9
ring/chain nodes :
12  14  15
chain bonds :
7-10  8-16  10-11  11-12  11-13
ring/chain bonds :
12-14  12-15
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  5-7  6-9  7-8  8-9
exact/norm bonds :
5-7  6-9  7-8  8-9  11-12  11-13  12-14  12-15
exact bonds :
7-10  8-16  10-11
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6

Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:Atom  8:Atom  9:Atom  10:CLASS
11:CLASS  12:CLASS  13:CLASS  14:CLASS  15:CLASS  16:CLASS  17:CLASS  18:Atom


L1      STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1                STR
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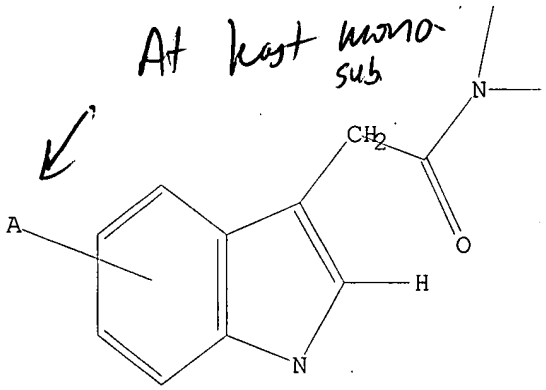
Claim 28

formula XII

At least mono-sub

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Structure attributes must be viewed using STN Express query preparation.

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FULL SEARCH INITIATED 12:53:47 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    39611 TO ITERATE

100.0% PROCESSED    39611 ITERATIONS                 122 ANSWERS
SEARCH TIME: 00.00.01

L2          122 SEA SSS FUL L1
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=> fil caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                              172.10     172.31

FILE 'CAPLUS' ENTERED AT 12:53:51 ON 20 FEB 2007
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 20 Feb 2007  VOL 146 ISS 9
FILE LAST UPDATED: 19 Feb 2007  (20070219/ED)

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http://www.cas.org/infopolicy.html

=> s l2
L3          69 L2

=> d ibib abs hitstr 1-69
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L3 ANSWER 1 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1286256 CAPLUS
DOCUMENT NUMBER: 146:45728
TITLE: Preparation of proline stilbenediamine amides and related compounds as inhibitors of HCV replication
INVENTOR(S): Serrano-Wu, Michael; Belema, Makonen; Snyder, Lawrence B.; Meanwell, Nicholas A.; St. Laurent, Denis R.; Kakarla, Ramesh; Nguyen, Van N.; Qiu, Yuping; Yang, Xuejie; Leet, John E.; Gao, Min; O'Boyle, Donald R.; Lemm, Julie A.; Yang, Fukang
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 156pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2006276511	A1	20061207	US 2006-446788	20060605
WO 2006133326	A1	20061214	WO 2006-US22197	20060606

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2005-687760P P 20050606

OTHER SOURCE(S): MARPAT 146:45728
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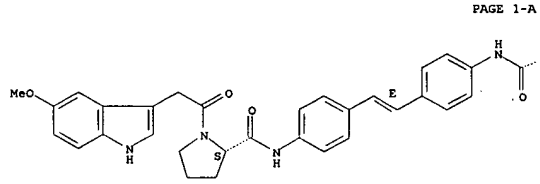
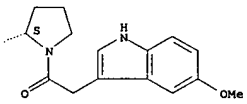


PAGE 1-A



PAGE 1-B

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to compds. I [m, n are 0-3; p is 0 or 1; X, Y are independently O, CH, CH2, CHR3, CR3; R1, R2 are independently alkoxy, alkyl, aryl, arylcarbonyl, cycloalkyl, heterocyclyl, amino groups, etc.; R3, R4 are independently H, alkoxy, alkoxycarbonyloxy, alkyl, alkylsulfonyl, aryl, azido, OH, amino groups, etc.; R5, R5 are independently H, alkenyl, alkoxycarbonyl, alkyl, alkylcarbonyl, aryl, arylalkyl, heterocyclylalkylcarbonyl, heterocyclylcarbonyl; R7, R8 are independently H, alkenyl, alkoxy, alkyl, halo, haloalkyl] which can inhibit hepatitis C virus (HCV) replication and in particular can inhibit the function of the HCV NS5A protein. Thus, compound II was prepared by amidation reaction and showed EC50 <0.050 μM against wild-type replicon

L3 ANSWER 1 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
cells.
IT 916443-93-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of proline stilbenediamine amides and related compds. as inhibitors of HCV replication)
RN 916443-93-1 CAPLUS
CN 2-Pyrrolidinecarboxamide, N,N'-[(1E)-1,2-ethenediyldi-4,1-phenylene]bis[1-[2-(5-methoxy-1H-indol-3-yl)acetyl]-, (2S,2'S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

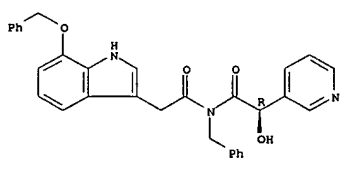
L3 ANSWER 2 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1228649 CAPLUS
DOCUMENT NUMBER: 145:505339
TITLE: Preparation of 2-(1-arylalkylamino)-1-pyridylethanol dihydrochloride hydrates
INVENTOR(S): Tanaka, Masahiko; Nakamura, Akihiko
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan; Dainippon Pharmaceutical Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 11pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006315992	A	20061124	JP 2005-139419	20050512

PRIORITY APPLN. INFO.: JP 2005-139419 20050512

OTHER SOURCE(S): MARPAT 145:505339
AB The hydrates QCH(OH)CH2NHR.2HCl.nH2O (Q = pyridyl; R = lower 1-arylalkyl; n = 0.5-1.5), useful as substitutes for moisture-absorbing 2-(1-arylalkylamino)-1-pyridylethanol hydrochlorides, are prepared by treatment of QCH(OH)CH2NHR.2HCl (Q, R = same as above) with H2O or treatment of QCH(OH)CH2NHR (Q, R = same as above) with HCl. Thus, 2-benzylamino-1-(3-pyridyl)ethanol (I) was treated with 35% HCl in THF/MeOH to give 95% I.2HCl.0.92H2O.
IT 915099-05-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (arylalkylamino)pyridylethanol dihydrochloride hydrates as substitutes for moisture-absorbing (arylalkylamino)pyridylethanol hydrochlorides)
RN 915099-05-7 CAPLUS
CN 1H-Indole-3-acetamide, N-[(2R)-hydroxy-3-pyridinylacetyl]-7-(phenylmethoxy)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 3 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:703152 CAPLUS
DOCUMENT NUMBER: 145:145754
TITLE: Preparation of indole derivatives as intermediates for β3-adrenoceptor agonists
INVENTOR(S): Umezome, Takashi; Yokoyama, Tatsuo
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan; Sumitomo Chemical Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 34 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006188505	A	20060720	JP 2005-355247	20051208

PRIORITY APPLN. INFO.: JP 2004-359139 A 20041210

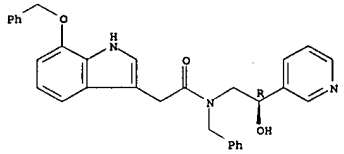
OTHER SOURCE(S): MARPAT 145:145754
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Indole derivs. I [Z = CH2; R1, R4 = H, (un)substituted alkyl, (un)substituted alkoxy, protected OH, protected NH2; number of R1 and R4 ≥1; R2 = H, (un)substituted alkyl, N-protecting group; R3 = OH-protecting group; R5 = H, (un)substituted alkyl; R6 = H, OH-protecting group; R8 = amino-protecting group; R13, R14 = H, (un)substituted alkyl] are prepared by (1) reaction of (carboxymethyl)indoles II (R1-R3, R13, R14 = same as above) with (aminoethyl)pyridines III (R4-R6, R8 = same as above) using condensing agents or by (1') reaction of halides or anhydrides of II with III and optional deprotection and (2) reduction of the resulting I (Z = CO; R1-R6, R8, R13, R14 = same as above). (morpholinocarbonylmethoxy)indoles I [Z = CR11R12; R1, R2, R4, R5, R8, R13, R14 = same as above; R3 = Q; R6 = H; R9-R12 = H, (un)substituted alkyl; number or R10 ≥1], which can be converted into I [Z = CR11R12; R1, R4, R5, R9, R11-R14 = same as above; R2, R6, R8 = H; R3 = CHR9CO2H] as β3-adrenoceptor agonists, are prepared by deprotecting I (Z = CR11R12; R1, R2, R4, R5, R8, R11-R14 = same as above; R3 = OH-protecting group; R6 = H) and reacting the resulting I (Z = CR11R12; .R1, R2, R4, R5, R8, R11-R14 = same as above; R3 = R6 = H) with morpholine derivs. IV (R9, R10 = same as above; X1 = leaving group) in the presence of bases. Thus, (2R)-N-benzyl-2-triethylsilyloxy-2-(3-pyridyl)ethylamine (preparation given) was reacted with {7-(benzyloxy)-1H-indol-3-yl}acetic acid in DMF in the presence of 1-hydroxybenzotriazole and 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide at 20-25° for 15 h to give 95% N-benzyl-2-{7-(benzyloxy)-1H-indol-3-yl}-N-[(2R)-2-hydroxy-2-pyridin-3-ylethyl]acetamide. A THF solution of

L3 ANSWER 3 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
amide was added dropwise to a THF suspension of LiAlH4 and the reaction mixt. was stirred at 20-25° for 3 h to give 83% (1R)-2-[benzyl[2-[7-(benzyloxy)-1H-indol-3-yl]ethyl]amino]-1-pyridin-3-ylethanol.
IT 898541-11-2P
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indole derivs. as intermediates for β3-adrenoceptor agonists)
RN 898541-11-2 CAPLUS
CN 1H-Indole-3-acetamide, N-[(2R)-2-hydroxy-2-(3-pyridinyl)ethyl]-7-(phenylmethoxy)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 4 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L3 ANSWER 4 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:600233 CAPLUS
DOCUMENT NUMBER: 145:293206
TITLE: Application of the Rh(II) Cyclization/Cycloaddition Cascade for the Total Synthesis of (±)-Aspidophytine
AUTHOR(S): Mejia-Oneto, Jose M.; Padwa, Albert
CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA
SOURCE: Organic Letters (2006), 8(15), 3275-3278
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:293206
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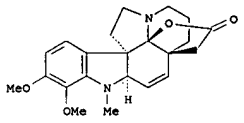
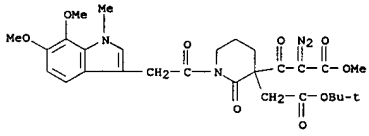


I

AB A new strategy for the synthesis of (±)-aspidophytine (I) has been developed and is based on a Rh(II)-catalyzed cyclization/dipolar cycloaddn. sequence. The resulting [3+2]-cycloadduct undergoes an efficient Lewis acid mediated cascade that rapidly provides the complete skeleton of aspidophytine. The synthesis also features a mild decarbomethoxylation reaction.
IT 908003-65-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(total synthesis of (±)-aspidophytine via the rhodium-catalyzed cyclization/cycloaddn. cascade)
RN 908003-65-6 CAPLUS
CN 3-Piperidinepropanoic acid, α-diazo-1-[(6,7-dimethoxy-1-methyl-1H-indol-3-yl)acetyl]-3-[2-(1,1-dimethylethoxy)-2-oxoethyl]-β,2-dioxo-, methyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 5 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:269508 CAPLUS
DOCUMENT NUMBER: 144:331420
TITLE: Preparation of bicyclic anilide spirolactam cgrp receptor antagonists
INVENTOR(S): Bell, Ian M.; Theberge, Cory R.; Stump, Craig A.; Zhang, Xufang; Gallicchio, Steven N.; Zartman, C. Blair
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006031610	A2	20060323	WO 2005-US32041	20050909
WO 2006031610	A3	20060831		

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RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-609292P P 20040913

OTHER SOURCE(S): MARPAT 144:331420
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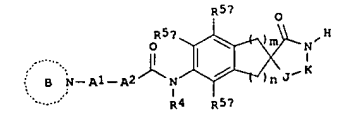

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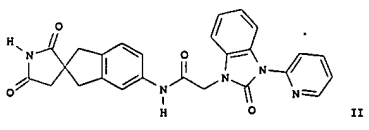


II

L3 ANSWER 5 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Title compds. I [A1 and A2 independently = bond or CR13R14, where one of A1 and A2 is optionally absent; B = (un)substituted bicycloheterocycle; J = =C(R6a)-; CR13R14, and CO; K = =C(R6b), CR13R14, CO, etc.; R4 = H, (un)substituted alkyl, benzyl, etc.; R5a, R5b, and R5c = H, alkyl, alkoxy, halo, etc.; R6a and R6b independently = H, OH, halo, (un)substituted alkyl, etc.; R13 and R14 = H or (un)substituted alkyl; m = 1 or 2; n = 1 or 2], and their pharmaceutically acceptable salts, useful as antagonists of calcitonin gene-related peptide (CGRP) receptors and useful in the treatment or prevention of diseases in which the CGRP is involved, such as headache, migraine and cluster headache. Thus, e.g., II was prepared by reaction of 5-amino-1,3-dihydro-2'H,5'H-spiro[indene-2,3'-pyrrolidine]-2',5'-dione (preparation given) with 5-amino-1,3-dihydrospiro[indene-2,3'-pyrrolo[2,3-b]pyridin]-2'(1'H)-one (preparation given). I demonstrated activity as antagonists of the CGRP receptor with Ki or IC50 values generally less than about 50 μM. The invention is also directed to pharmaceutical compns. comprising these compds. and the use of these compds. and compns. in the prevention or treatment of such diseases in which CGRP is involved.

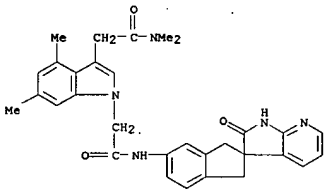
IT 880078-71-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of bicyclic anilide spirolactam cgrp receptor antagonists)

RN 880078-71-7 CAPLUS

CN 1H-Indole-1,3-diacetamide, N3,N3,4,6-tetramethyl-N1-(1,1',2',3-tetrahydro-2'-oxospiro[2H-indene-2,3'-[3H]pyrrolo[2,3-b]pyridin]-5-yl)- (9CI) (CA INDEX NAME)



L3 ANSWER 6 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:325699 CAPLUS

DOCUMENT NUMBER: 142:392292

TITLE: Preparation of heterocyclic compounds, e.g., N-alkylpiperidin-3-yl substituted analogs as ligands for monoamine receptors and transporters for treating drug addiction or drug dependence

INVENTOR(S): Aquila, Brian M.; Bannister, Thomas D.; Cuny, Gregory D.; Hauske, James R.; Holland, Joanne M.; Persons, Paul E.; Radeke, Heike S.; Wang, Fengjiang; Shao, Liming

PATENT ASSIGNEE(S): Sepracor, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 161 pp., Cont.-in-part of U.S. Ser. No. 607,457.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005080078	A1	20050414	US 2004-771519	20040204
US 2003050309	A1	20030313	US 2001-951130	20010912
US 2004077706	A1	20040422	US 2003-607457	20030626
US 7132551	B2	20061107		
WO 2005077463	A2	20050825	WO 2005-US3629	20050204
WO 2005077463	A3	20060126		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, SM

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:

US 2001-273530P	P	20010305
US 2001-298057P	P	20010613
US 2001-951130	A3	20010912
US 2003-607457	A2	20030626
US 2000-231667P	P	20000911
US 2004-771519	A	20040204

OTHER SOURCE(S): MARPAT 142:392292

GI

L3 ANSWER 6 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. (4 Markush structures given), e.g., I [X = C(R3)2, O, SO0-2, NR2, NC(O)R7, NC(O)OR2, NS(O)2R7, C=O; Z = C(R3)2, C(O), O, NR, NC(O)OR, SO0-2; m = 1-5; n = 1-2; p = 0-2; q = 0-3; R = H, (cyclo)alkyl, (hetero)aryl, aralkyl, heteroaralkyl; R1 = H, alkyl, (hetero)aryl, aralkyl, heteroaralkyl; R, R1 may be connected through a covalent bond; R2 = H, alkyl, fluoroalkyl, aryl, heteroaryl, cycloalkyl; R3 = H, alkyl, aryl, OR2, OC(O)R2, CH2OR2, CO2R2; wherein any two instances of R3 may be connected by a covalent tether whose backbone consists of 1, 2, 3, or 4-carbon atoms; R4 = H, alkyl, cycloalkyl, aryl, heteroaryl, alkenyl, OR; R5-6 = H, alkyl, (CH2)qY, aryl, heteroaryl, F, OR2, OC(O)R2, or an instance of CR5R6 taken together is C(O); R7 = (cyclo)alkyl, (hetero)aryl, aralkyl, or heteroaralkyl; R8-9 = H, alkyl, (CH2)qY, (hetero)aryl, F, OR2, OC(O)R2, or an instance of CR8R9 taken together is C(O); Y = OR2, N(R2)2, SO0-2R2, P(O)(OR2)2; any two instances of R2 may be connected through a covalent bond; a covalent bond may connect R4 and an instance of R5 or R6; any two instances of R5 and R6 may be connected through a covalent bond; any two geminal or vicinal instances of R8 and R9 may be connected through a covalent bond; and the stereochem. configuration at any stereocenter of I is R, S or a mixture of these configurations.] were prepared Examples include synthesis of several hundred compds. of structure I, functional assays for norepinephrine (NE), dopamine (DA) and serotonin (5-HT) antagonism, determination of NE, DA and 5-HT reuptake inhibition, spontaneous locomotor activity/antidepressant behavioral assay in rats and the synthesis of a 96-member combinatorial library in which the library compds. were screened for monoamine uptake inhibition. For instance, 3-((4-trifluoromethylphenoxy)methyl)piperidine trifluoroacetate was alkylated with 1-[(4-chlorophenyl)cyclobutyl]-2-chloroethanone (preparation given) and the resulting product reduced with NaBH4 to give II. All 4 enantiomers of II were prepared by a stereospecific synthesis, and X-ray crystallog. determination of one enantiomer allowed the absolute stereochem. of III to be assigned. III had EC50 < 10 nM for DA reuptake inhibition compared to nomifensine = 11 nM. I are useful for the treatment of cocaine addiction or methamphetamine addiction.

IT 405089-92-1P

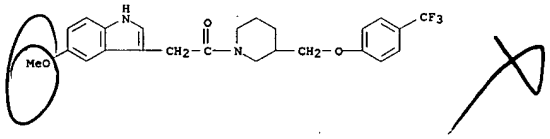
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclic compds., e.g., N-alkylpiperidin-3-yl substituted analogs as ligands for monoamine receptors and transporters)

RN 405089-92-1 CAPLUS

CN Piperidine, 1-[(5-methoxy-1H-indol-3-yl)acetyl]-3-[[4-(trifluoromethyl)phenoxy]methyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 6 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L3 ANSWER 7 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:902086 CAPLUS
DOCUMENT NUMBER: 141:388753
TITLE: Heterocyclic compound modulators of Tie-2 and other kinases, and therapeutic use
INVENTOR(S): Chen, Jeff; Dalrymple, Lisa; Epshteyn, Sergery; Forsyth, Timothy; Huynh, Tai; Leahy, James; Mann, Grace; Mann, Larry W.; Ridgway, Brian; Sangalang, Joan C.; Takeuchi, Craig
PATENT ASSIGNEE(S): Exelixis, Inc., USA
SOURCE: PCT Int. Appl., 126 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004091480	A2	20041028	WO 2004-US10626	20040408
WO 2004091480	A3	20050811		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004229392	A1	20041028	AU 2004-229392	20040408
CA 2520255	A1	20041028	CA 2004-2520255	20040408
EP 1611123	A2	20060104	EP 2004-759191	20040408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2006522813	T	20061005	JP 2006-509755	20040408
US 2006293342	A1	20061228	US 2006-552424	20060705

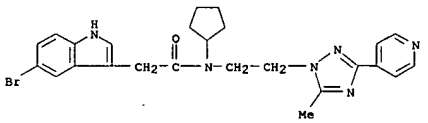
PRIORITY APPLN. INFO.: US 2003-461471P P 20030409
WO 2004-US10626 A 20040408

OTHER SOURCE(S): MARPAT 141:388753

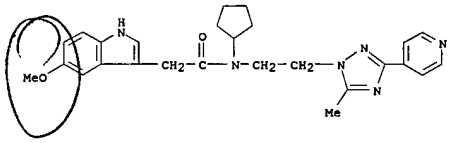
AB The invention provides heterocyclic compds. for modulating protein kinase enzymic activity for modulating cellular activities such as proliferation, differentiation, programmed cell death, migration and chemoinvasion. Compds. of the invention inhibit, regulate and/or modulate kinases, particularly Tie-2. Methods of using the compds. and pharmaceutical compns. thereof to treat kinase-dependent diseases and conditions are also an aspect of the invention. Preparation of triazolyl compds. of the invention is included.

IT 783330-82-5 783330-83-6
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(heterocyclic compound modulators of Tie-2 and other kinases, and therapeutic use)

RN 783330-82-5 CAPLUS
CN 1H-Indole-3-acetamide, 5-bromo-N-cyclopentyl-N-[2-[5-methyl-3-(4-pyridinyl)-1H-1,2,4-triazol-1-yl]ethyl]- (9CI) (CA INDEX NAME)



RN 783330-83-6 CAPLUS
CN 1H-Indole-3-acetamide, N-cyclopentyl-5-methoxy-N-[2-[5-methyl-3-(4-pyridinyl)-1H-1,2,4-triazol-1-yl]ethyl]- (9CI) (CA INDEX NAME)

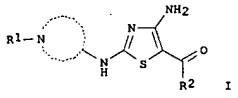


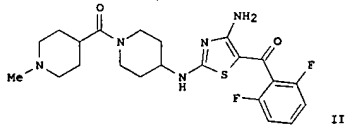
L3 ANSWER 8 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:718536 CAPLUS
DOCUMENT NUMBER: 141:243546
TITLE: Preparation of N-heterocyclyl-substituted amino-thiazole derivatives as protein kinase inhibitors
INVENTOR(S): Alegria, Larry Andrew; Chong, Wesley Kwan Mung; Chu, Shaosong; Duvadie, Rohit Kumar; Li, Lin; Romines, William Henry, III; Yang, Yi
PATENT ASSIGNEE(S): Pfizer Inc., USA
SOURCE: PCT Int. Appl., 307 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004074283	A1	20040902	WO 2004-IB433	20040209
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2516234	A1	20040902	CA 2004-2516234	20040209
EP 1597256	A1	20051123	EP 2004-709302	20040209
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2004007618	A	20060221	BR 2004-7618	20040209
JP 2006518368	T	20060810	JP 2006-502453	20040209
US 2005101595	A1	20050512	US 2004-783887	20040220

PRIORITY APPLN. INFO.: US 2003-448843P P 20030221
WO 2004-IB433 W 20040209

OTHER SOURCE(S): MARPAT 141:243546
GI



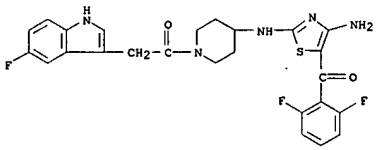


AB The title aminothiazole compds. with N-containing cycloalkyl at the 2-amino position [I; N-containing heterocyclyl = (un)substituted N-containing 3-10 membered heterocyclyl; R1 = H, alkyl, alkenyl, alkoxy, etc.; R2 = (un)substituted alkyl, cycloalkyl, alkoxy, aryl, 4-10 membered heterocyclyl] and their pharmaceutically acceptable prodrugs or salts which modulate and/or inhibit the cell proliferation and activity of protein kinases, were prepared Thus, reacting [4-amino-2-(piperidin-4-ylamino)thiazol-5-yl](2,6-difluorophenyl)methanone (preparation given) with 1-methylpiperidine-4-carboxylic acid afforded 65% II which showed Ki of 0.46 μM against CDK2, Ki of 0.13 μM against CDK4, and IC50 of >5 μM in HCT-116 assay for cell growth inhibition. Biol. data were given for over 1100 compds. I. The pharmaceutical compns. comprising the compound I are claimed.

IT 750582-26-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-heterocyclyl-substituted amino-thiazole derivs. as protein kinase inhibitors)

RN 750582-26-4 CAPLUS
CN 4-Piperidinamine, N-[4-amino-5-(2,6-difluorobenzoyl)-2-thiazolyl]-1-[(5-fluoro-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 8 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

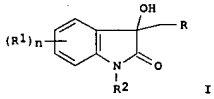
L3 ANSWER 9 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:546477 CAPLUS
DOCUMENT NUMBER: 141:89009
TITLE: Synthesis of tryptamine derivatives and intermediates thereof
INVENTOR(S): Berens, Ulrich; Dosenbach, Oliver; Sprenger, Daniel
PATENT ASSIGNEE(S): Ciba Specialty Chemicals Holding Inc., Switz.
SOURCE: PCT Int. Appl., 84 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004056769	A2	20040708	WO 2003-EP50992	20031212
WO 2004056769	A3	20040916		
WO 2004056769	B1	20041104		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2508290	A1	20040708	CA 2003-2508290	20031212
AU 2003299227	A1	20040714	AU 2003-299227	20031212
EP 1572647	A2	20050914	EP 2003-799560	20031212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1729174	A	20060201	CN 2003-80107086	20031212
JP 2006516128	T	20060622	JP 2004-561492	20031212
US 2006058367	A1	20060316	US 2005-539151	20050616

PRIORITY APPLN. INFO.: EP 2002-406128 A 20021220
WO 2003-EP50992 W 20031212

OTHER SOURCE(S): MARPAT 141:89009
GI



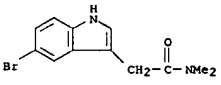
I

L3 ANSWER 9 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

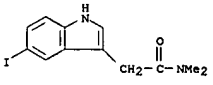
AB Indoleacetates I [R = CO2R3; R1 = (un)substituted alkyl, aryl, heterocyclyl, alkylsulfonyl, OH, SH, NO2, halogen, CN, CONH2, CONHNH2, CO2H, alkenyl, alkynyl, cycloalkyl, acyloxy, NH2, NHNH2, B(OH)2; R2 = H, (un)substituted alkyl, CO2H, arylsulfonyl, alkylsulfonyl, aryl, CONH2, silyl; R3 = (un)substituted alkyl; n = 0-4] were prepared and converted to I [R = CONR4R5; R4, R5 = (un)substituted alkyl; R4R5 = (un)substituted alkylene] which were in turn converted to indoleacetamides and tryptamines. The synthesis methods and products are useful in the synthesis of pharmaceuticals. Thus, 5-bromoisatin was treated with CH2(CO2H)2 and ClCONMe2 to give I [R = CONMe2, R1 = 5-Br, R2 = H] which was treated with BF3.Et2O and BH3.Me2SO to give 2-(5-bromo-1H-indol-3-yl)-N,N-dimethylacetamide or with BF3.Et2O and NaBH4 to give [2-(5-bromo-1H-indol-3-yl)ethyl]-N,N-dimethylacetamide.

IT 717139-79-2P 717139-83-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tryptamine derivs. and intermediates thereof)

RN 717139-79-2 CAPLUS
CN 1H-Indole-3-acetamide, 5-bromo-N,N-dimethyl- (9CI) (CA INDEX NAME)



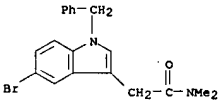
RN 717139-83-8 CAPLUS
CN 1H-Indole-3-acetamide, 5-iodo-N,N-dimethyl- (9CI) (CA INDEX NAME)



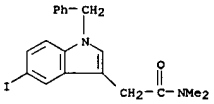
IT 717139-80-5P 717139-84-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of tryptamine derivs. and intermediates thereof)

RN 717139-80-5 CAPLUS
CN 1H-Indole-3-acetamide, 5-bromo-N,N-dimethyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 9 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 717139-84-9 CAPLUS
CN 1H-Indole-3-acetamide, 5-iodo-N,N-dimethyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



R1 = X

L3 ANSWER 10 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

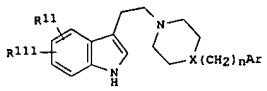
ACCESSION NUMBER: 2004:525891 CAPLUS
DOCUMENT NUMBER: 141:89110
TITLE: Preparation of piperazinylethylindolecarbonitriles as serotonin reuptake inhibitors and 5-HT1A/5-HT1B receptor ligands.
INVENTOR(S): Heinrich, Timo; Boettcher, Henning; Schiemann, Kai; Hoelzemann, Guenter; van Amsterdam, Christoph; Bartoszyk, Gerd; Leibrock, Joachim; Seyfried, Christoph
PATENT ASSIGNEE(S): Merck Patent GmbH, Germany
SOURCE: Ger. Offen., 23 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10259244	A1	20040701	DE 2002-10259244	20021217
CA 2510169	A1	20040701	CA 2003-2510169	20031127
WO 2004054972	A1	20040701	WO 2003-EP13374	20031127
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003298145	A1	20040709	AU 2003-298145	20031127
EP 1572646	A1	20050914	EP 2003-795848	20031127
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003017422	A	20051108	BR 2003-17422	20031127
CN 1729173	A	20060201	CN 2003-80106737	20031127
JP 2006511522	T	20060406	JP 2004-559727	20031127
US 2006122191	A1	20060608	US 2005-539516	20050617

PRIORITY APPLN. INFO.: DE 2002-10259244 A 20021217
WO 2003-EP13374 W 20031127

OTHER SOURCE(S): MARPAT 141:89110
GI

L3 ANSWER 10 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

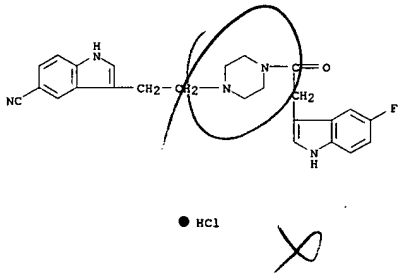


I

AB Title compds. [I; R11, R111 = H, cyano, halo, A, OA, OH, COR2, CH2R2; R2 = OH, OA, NH2, NHA, NA2; A = (fluoro-substituted) alkyl optionally interrupted by O, S, CH:CH; Ar = (partially or completely saturated) (substituted) mono- or polycyclic carbo- or heterocyclyl; n = 0-4], were prepared Thus, 3-(2-chloroeth-1-yl)-1H-indole-5-carbonitrile (preparation given), 1-(2,3-dihydrobenzo[1,4]-dioxin-5-yl)piperazine, ethyldiisopropylamine, and N-methylpyrrolidinone were heated together at 120° for 12 h to give 3-[2-[4-(2,3-dihydrobenzo[1,4]dioxin-5-yl)piperazin-1-yl]ethyl]-1H-indole-5-carbonitrile. The latter showed SSRI, 5-HT1A, and 5-HT1B receptor activity at 11 nM, 17 nM, and 11 nM, resp.

IT 714954-07-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of piperazinylethylindolecarbonitriles as serotonin reuptake inhibitors and receptor ligands)

RN 714954-07-1 CAPLUS
CN Piperazine, 1-[2-(5-cyano-1H-indol-3-yl)ethyl]-4-[(5-fluoro-1H-indol-3-yl)acetyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L3 ANSWER 11 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

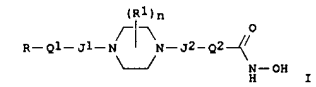
ACCESSION NUMBER: 2003:796490 CAPLUS
DOCUMENT NUMBER: 139:307794
TITLE: Preparation of N-hydroxy (piperazinesulfonyl)- or (piperazinecarbonyl)arylpropenamides as inhibitors of histone deacetylase and antiproliferative agents for the treatment of cancer and psoriasis
INVENTOR(S): Watkins, Clare J.; Romero-Martin, Maria-Rosario; Ritchie, James; Finn, Paul W.; Kalvinsh, Ivars; Loza, Einars; Dikovska, Klara; Starchenkov, Igor; Lolya, Daina; Gailite, Vjia
PATENT ASSIGNEE(S): Prolifix Limited, UK
SOURCE: PCT Int. Appl., 217 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003082288	A1	20031009	WO 2003-GB1463	20030403
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2479906	A1	20031009	CA 2003-2479906	20030403
AU 2003229883	A1	20031013	AU 2003-229883	20030403
BR 2003008908	A	20050104	BR 2003-8908	20030403
EP 1492534	A1	20050105	EP 2003-722719	20030403
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005143385	A1	20050630	US 2003-509732	20030403
JP 2005527556	T	20050915	JP 2003-579825	20030403
NO 2004004744	A	20041102	NO 2004-4744	20041102

PRIORITY APPLN. INFO.: US 2002-369337P P 20020403
WO 2003-GB1463 W 20030403

OTHER SOURCE(S): MARPAT 139:307794
GI

L3 ANSWER 11 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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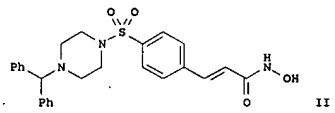


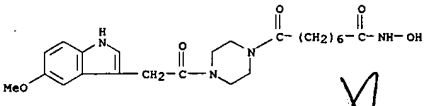
II

AB N-hydroxyamides I [J1 = single bond, C(:O), J2 = C(:O), SO2; Q1 = single bond, OX, SX, XOY, XSY, XO, XS; Q2 = (un)substituted C4-C8 alkylene at least four carbon atoms in length; R = (un)substituted cycloalkyl, heterocycloalkyl, or aryl; R1 = C1-C4 alkyl; X, Y = (un)substituted alkanediyl; n = 0-8] containing piperazine moieties, particularly N-hydroxy piperazinesulfonylarylpropenamides such as II, are prepared as inhibitors of histone deacetylase (HDAC) for the treatment of proliferative diseases, cancer, and psoriasis in both humans and animals. Biol. data on the inhibition of HDAC in vitro, the inhibition of cellular proliferation in vitro, and the in vivo testing of I on mice containing i.p. P388 tumors are given for a subset of I. Most of the compds. I tested inhibit HDAC with IC50 values between 20 nM and 200 nM, inhibit proliferation of four cell lines with IC50 values between 1 μM and 10 μM, and give log rank statistics for mice with P388 tumors (5 each) of between -3 and -5. II gives a log rank statistic for tumors in five mice of -9.62. Preparative data for approx. fifty of the title compds. are given.

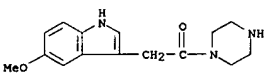
IT 610801-57-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compds.; preparation of N-hydroxy (piperazinesulfonyl)- or (piperazinecarbonyl)arylpropenamides as inhibitors of histone deacetylase and antiproliferative agents for the treatment of cancer and psoriasis)

RN 610801-57-5 CAPLUS
CN 1-Piperazineoctanamide, N-hydroxy-4-[(5-methoxy-1H-indol-3-yl)acetyl]-η-oxo- (9CI) (CA INDEX NAME)

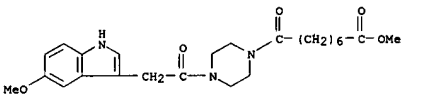
L3 ANSWER 11 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 610802-13-6P 610802-39-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediates; preparation of N-hydroxy (piperazinesulfonyl)- or (piperazinecarbonyl)arylpropenamides as inhibitors of histone deacetylase and antiproliferative agents for the treatment of cancer and psoriasis)
RN 610802-13-6 CAPLUS
CN Piperazine, 1-[(5-methoxy-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)



RN 610802-39-6 CAPLUS
CN 1-Piperazineoctanoic acid, 4-[(5-methoxy-1H-indol-3-yl)acetyl]-η-oxo-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

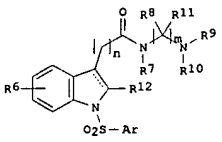
L3 ANSWER 12 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:656572 CAPLUS
DOCUMENT NUMBER: 139:197363
TITLE: Preparation of 1-arylsulfonyl-3-substituted indoles and indolines for the treatment of central nervous system disorders
INVENTOR(S): Spinks, Daniel; Armer, Richard E.; Miller, David J.; Rankovic, Zoran; Spinks, Gayle; Mestres, Jordi; Jaap, David Robert
PATENT ASSIGNEE(S): Akzo Nobel N.V., Neth.
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003068220	A1	20030821	WO 2003-EP50010	20030205
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003208711	A1	20030904	AU 2003-208711	20030205
EP 1476151	A1	20041117	EP 2003-706618	20030205
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005154023	A1	20050714	US 2003-504556	20030205
JP 2005526033	T	20050902	JP 2003-567402	20030205
PRIORITY APPLN. INFO.:			EP 2002-75584 A	20020212
			WO 2003-EP50010 W	20030205

OTHER SOURCE(S): MARPAT 139:197363
GI

L3 ANSWER 12 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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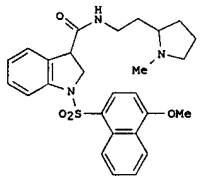
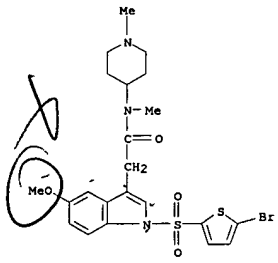


II

AB The title compds. [I; Ar = (un)substituted (hetero)aryl; n = 0-1; m = 0-5;
R6 = H, alkyl, alkoxy, etc.; R7 = H, alkyl, aryl, arylalkyl; or R7 together with R9 or with one of R8 forms 4-7 membered saturated ring; R8 = H,
alkyl, aryl; or one of R8 together with R7 or R9 or the geminal R11 forms 4-7 membered saturated ring, and other R8 = H, alkyl or (un)substituted aryl;
R9, R10 = H, alkyl, aryl, arylalkyl; or NR9R10 = 5-7 membered (un)saturated
ring optionally containing O or N atoms; R11 = H, alkyl; or one of R11 together with R10 or with the geminal R8 forms 4-7 membered saturated ring,
and the other R11 = H, alkyl], useful in the treatment of central nervous disorders such as psychosis, schizophrenia, manic depressions, depressions, neurol. disorders, cognitive enhancement, Parkinson' s disease, amyotrophic lateral sclerosis, Alzheimer' s disease and Huntington' s disease, were prepared E.g., a 4-step synthesis of II (starting from 1H-indole-3-carboxylic acid) which showed pKi of > 7.5 against 5-HT6 receptor binding, was given. Pharmaceutical composition comprising the compound I is claimed.
IT 583814-43-1P 583814-57-7P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-arylsulfonyl-3-substituted indoles and indolines for the
treatment of central nervous system disorders)
RN 583814-43-1 CAPLUS
CN 1H-Indole-3-acetamide, 1-[(5-bromo-2-thienyl)sulfonyl]-5-methoxy-N-methyl-N-(1-methyl-4-piperidinyl)-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 583814-42-0
CMF C22 H26 Br N3 O4 S2



CM 2

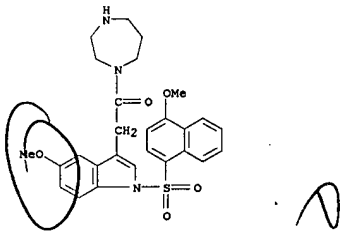
CRN 76-05-1
CMF C2 H F3 O2

RN 583814-57-7 CAPLUS
CN 1H-1,4-Diazepine, hexahydro-1-[[5-methoxy-1-[(4-methoxy-1-naphthalenyl)sulfonyl]-1H-indol-3-yl]acetyl]-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 583814-56-6
CMF C27 H29 N3 O5 S

L3 ANSWER 12 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

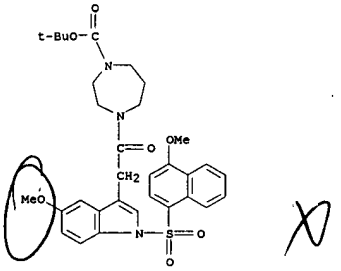


CM 2

CRN 76-05-1
CMF C2 H F3 O2

IT 583815-11-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1-arylsulfonyl-3-substituted indoles and indolines for the
treatment of central nervous system disorders)
RN 583815-11-6 CAPLUS
CN 1H-1,4-Diazepine-1-carboxylic acid, hexahydro-4-[[5-methoxy-1-[(4-methoxy-1-naphthalenyl)sulfonyl]-1H-indol-3-yl]acetyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

L3 ANSWER 12 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L3 ANSWER 13 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:319488 CAPLUS
DOCUMENT NUMBER: 138:337988
TITLE: Novel 2-[(iminomethyl)amino]phenyl derivatives useful as inhibitors of NO synthase and lipid peroxidation, their preparation, their application as medicines, and pharmaceutical compositions containing them
INVENTOR(S): Chabrier De Lassauniere, Pierre Etienne; Auvin, Serge; Bigg, Dennis; Auguet, Michel; Harnett, Jeremiah
PATENT ASSIGNEE(S): Societe de Conseils de Recherches et D'Applications scientifiques (S.C.R.A.S.), Fr.
SOURCE: U.S. Pat. Appl. Publ., 78 pp., Cont.-in-part of U.S. Ser. No. 882,264.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003078420	A1	20030424	US 2002-191950	20020709
US 6809088	B2	20041026		
FR 2761066	A1	19980925	FR 1997-3528	19970324
FR 2761066	B1	20001124		
FR 2764889	A1	19981224	FR 1997-7701	19970620
FR 2764889	B1	20000901		
WO 9842696	A1	19981001	WO 1998-FR288	19980216
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
WO 9858934	A1	19981230	WO 1998-FR1250	19980615
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6335445	B1	20020101	US 1999-456205	19991207
US 2002007062	A1	20020117	US 2001-882264	20010615
US 6630461	B2	20031007		
US 2005043397	A1	20050224	US 2004-898916	20040726
US 7122535	B2	20061017		
US 2005187272	A1	20050825	US 2005-105291	20050413

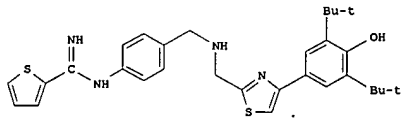
PRIORITY APPLN. INFO.:

FR 1997-3528	A	19970324
FR 1997-7701	A	19970620
WO 1998-FR288	W	19980216
WO 1998-FR1250	W	19980615

L3 ANSWER 13 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

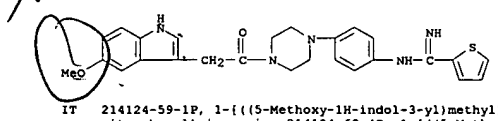
US 1999-456205	A3	19991207
US 2001-882264	A2	20010615
US 1999-381749	A2	19990922
US 2002-191950	A3	20020709
US 2004-898916	A3	20040726

OTHER SOURCE(S): MARPAT 138:337988
GI



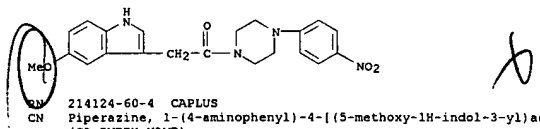
I

AB Title compds., e.g., N-[4-[[[[4-(3,5-di-tert-butyl-4-hydroxyphenyl)-1,3-thiazol-2-yl]methyl]amino]methyl]phenyl]thiophene-2-carboximidamide (I) are prepared The compds. are inhibitors of NO synthases, and are also antioxidants which inhibit lipid peroxidn. Approx. 70 examples are prepared
I had IC50 for inhibiting rat neuronal NO synthase in vitro < 3.5 μM, and the IC50 for inhibiting rat cerebral lipid peroxidn. in vitro is < 30 μM.
IT 214123-85-0P, N-[4-[4-[((5-Methoxy-1H-indol-3-yl)methyl)carbonyl]-1-piperazinyl]phenyl]-2-thiophenecarboximidamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and testing of 2-[(iminomethyl)amino]phenyl derivs. as inhibitors of NO synthase and lipid peroxidn.)
RN 214123-85-0 CAPLUS
CN Piperazine, 1-[4-[(imino-2-thienylmethyl)amino]phenyl]-4-[(5-methoxy-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)

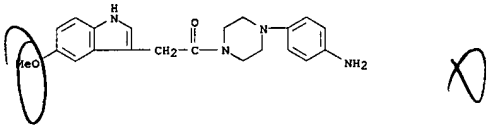


IT 214124-59-1P, 1-[((5-Methoxy-1H-indol-3-yl)methyl)carbonyl]-4-(4-nitrophenyl)piperazine 214124-60-4P, 1-[((5-Methoxy-1H-indol-3-yl)methyl)carbonyl]-4-(4-aminophenyl)piperazine
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and testing of 2-[(iminomethyl)amino]phenyl derivs. as inhibitors of NO synthase and lipid peroxidn.)

L3 ANSWER 13 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 214124-59-1 CAPLUS
CN Piperazine, 1-[(5-methoxy-1H-indol-3-yl)acetyl]-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 214124-60-4 CAPLUS
CN Piperazine, 1-(4-aminophenyl)-4-[(5-methoxy-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)

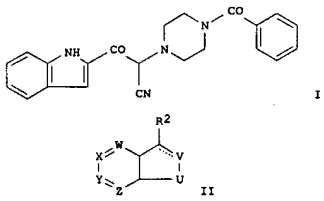


L3 ANSWER 14 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:832569 CAPLUS
DOCUMENT NUMBER: 137:337880
TITLE: Preparation of indole, azaindole, and related heterocyclic piperazinecarboxamides for treatment of AIDS
INVENTOR(S): Wang, Tao; Wallace, Owen B.; Meanwell, Nicholas A.; Zhang, Zhongxing; Bender, John A.; Kadow, John F.; Yeung, Kap-Sun
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002085301	A2	20021031	WO 2002-US12856	20020423
WO 2002085301	A3	20030227		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003096825	A1	20030522	US 2002-127256	20020422
US 6825201	B2	20041130		
CA 2445190	A1	20021031	CA 2002-2445190	20020423
EP 1381366	A2	20040121	EP 2002-764315	20020423
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2002009153	A	20040720	BR 2002-9153	20020423
CN 1520295	A	20040811	CN 2002-812629	20020423
JP 2004527538	T	20040909	JP 2002-582877	20020423
HU 200401503	A2	20041228	HU 2004-1503	20020423
PRIORITY APPLN. INFO.:			US 2001-286347P P	20010425
			WO 2002-US12856 W	20020423

OTHER SOURCE(S): MARPAT 137:337880
GI

L3 ANSWER 14 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I

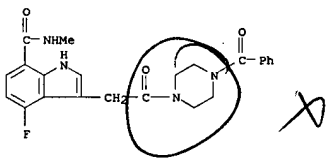
II

AB This invention provides indole, azaindole, and related heterocyclic piperazinecarboxamides Q(C(O))m(CR8R8')n(C(O))pTC(O)A (I; variables defined below; e.g. N-(benzoyl)-N'-[2-(indol-2-yl)-2-oxo-1-cyanoethyl]piperazine (shown as I)) having drug and bio-affecting properties, their pharmaceutical compns. and method of use. These compds. possess unique antiviral activity, whether used alone or in combination with other antivirals, antiinfectives, immunomodulators or HIV entry inhibitors. More particularly, the present invention relates to the treatment of HIV and AIDS. EC50 ranges against HIV-1 are given for about 30 of the claimed compds.; for example, N-(benzoyl)-N'-[2-(6-methoxyindol-2-yl)-2-oxo-1-cyanoethyl]-3-methylpiperazine has an EC50 <1μM. Although the methods of preparation are not claimed, 32 example prepns. of I and 6 example prepns. of intermediates are included. In I: Q is shown as II (dotted line may be a bond); A is C1-6alkoxy, C1-6alkyl, C3-7cycloalkyl, Ph, and heteroaryl; T is piperazine-1,4-diyl; U is NR7, O, or S; V is C(H)kR1, O or N(R7)k; W is CR3 or NR10; X is CR4 or NR10; Y is CR5 or NR10; Z is CR6 or NR10; k is 0 or 1; m, n, and p are 0-2 provided that the sum of m, n, and p must equal 1 or 2; R8 and R8 are H, hydroxy, C1-6alkyl, C1-6alkoxy, cyano, and fluoro, or R8 and R8' taken together form :O, :S, :NOR9, or :NH; other variables and provisos are given in the claims.

IT 474012-42-5P, 3-[2-(4-Benzoylpiperazin-1-yl)-2-oxoethyl]-4-fluoro-1H-indole-7-carboxylic acid methylamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of indole, azaindole, and related heterocyclic piperazinecarboxamides for treatment of AIDS)

RN 474012-42-5 CAPLUS
CN 1H-Indole-7-carboxamide, 3-[2-(4-benzoyl-1-piperazinyl)-2-oxoethyl]-4-fluoro-N-methyl- (9CI) (CA INDEX NAME)

L3 ANSWER 14 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



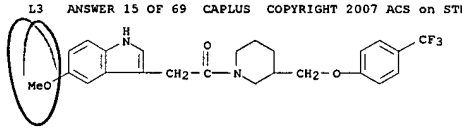
L3 ANSWER 15 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:220550 CAPLUS
DOCUMENT NUMBER: 136:263097
TITLE: Preparation of heterocyclic compounds, e.g., N-alkylpiperidin-3-yl substituted analogs as ligands for monoamine receptors and transporters.
INVENTOR(S): Aquila, Brian M.; Bannister, Thomas D.; Cuny, Gregory D.; Hauske, James R.; Holland, Joanne M.; Persons, Paul E.; Radeke, Heike; Wang, Fengjian; Shao, Liming
PATENT ASSIGNEE(S): Sepracor, Inc., USA
SOURCE: PCT Int. Appl., 275 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002022572	A2	20020321	WO 2001-US28654	20010912
WO 2002022572	A3	20020801		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2422055	A1	20020321	CA 2001-2422055	20010912
AU 2001090873	A5	20020326	AU 2001-90873	20010912
EP 1318988	A2	20030618	EP 2001-970926	20010912
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004509103	T	20040325	JP 2002-526825	20010912
PRIORITY APPLN. INFO.:			US 2000-231667P P	20000911
			US 2001-273530P P	20010305
			US 2001-298057P P	20010613
			US 2000-273530P P	20010305
			US 2000-298057P P	20010613
			WO 2001-US28654 W	20010912

OTHER SOURCE(S): MARPAT 136:263097
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L3 ANSWER 15 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L3 ANSWER 15 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Title compds. (4 Markush structures given), e.g., I [X = C(R3)2, O, SO0-2, NR2, NC(O)R7, NC(O)OR2, NS(O)2R7, C=O; Z = C(R3)2, C(O), O, NR, NC(O)OR, SO0-2; m = 1-5; n = 1-2; p = 0-2; q = 0-3; R = H, (cyclo)alkyl, (hetero)aryl, aralkyl, heteroaralkyl; R1 = H, alkyl, (hetero)aryl, aralkyl, heteroaralkyl; R, R1 may be connected through a covalent bond; R2 = H, alkyl, fluoroalkyl, aryl, heteroaryl, cycloalkyl; R3 = H, alkyl, aryl, OR2, OC(O)R2, CH2OR2, CO2R2; wherein any two instances of R3 may be connected by a covalent tether whose backbone consists of 1, 2, 3, or 4-carbon atoms; R4 = H, alkyl, cycloalkyl, aryl, heteroaryl, alkenyl, OR; R5-6 = H, alkyl, (CH2)qY, aryl, heteroaryl, F, OR2, OC(O)R2, or an instance of CR5R6 taken together is C(O); R7 = (cyclo)alkyl, (hetero)aryl, aralkyl, or heteroaralkyl; R8-9 = H, alkyl, (CH2)qY, (hetero)aryl, F, OR2, OC(O)R2, or an instance of CR8R9 taken together is C(O); Y = OR2, N(R2)2, SO0-2R2, P(O)(OR2)2; any two instances of R2 may be connected through a covalent bond; a covalent bond may connect R4 and an instance of R5 or R6; any two instances of R5 and R6 may be connected through a covalent bond; any two geminal or vicinal instances of R8 and R9 may be connected through a covalent bond; and the stereochem. configuration at any stereocenter of I is R, S or a mixture of these configurations.] were prepared Examples include synthesis of several hundred compds. of structure I, functional assays for norepinephrine (NE), dopamine (DA) and serotonin (5-HT) antagonism, determination of NE, DA and 5-HT reuptake inhibition, spontaneous locomotor activity/antidepressant behavioral assay in rats and the synthesis of a 96-member combinatorial library in which the library compds. were screened for monoamine uptake inhibition. For instance, 3-({4-trifluoromethylphenoxy)methyl)piperidine trifluoroacetate was alkylated with 1-[(4-chlorophenyl)cyclobutyl]-2-chloroethanone (preparation given) and the resulting product reduced with NaBH4 to give II. All 4 enantiomers of II were prepared by a stereospecific synthesis, and X-ray crystallog. determination of one enantiomer allowed the absolute stereochem. of III to be assigned. III had EC50 < 10 nM for DA reuptake inhibition compared to nomifensine = 11 nM. I are useful for the treatment of depression, sexual dysfunction, Alzheimer's disease, anxiety, etc.
IT 405089-92-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic compds., e.g., N-alkylpiperidin-3-yl substituted analogs as ligands for monoamine receptors and transporters)
RN 405089-92-1 CAPLUS
CN Piperidine, 1-[(5-methoxy-1H-indol-3-yl)acetyl]-3-[[4-(trifluoromethyl)phenoxy]methyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 16 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:172553 CAPLUS
DOCUMENT NUMBER: 136:355101
TITLE: Aromatization of 1,6,7,7a-Tetrahydro-2H-indol-2-ones by a Novel Process. Preparation of Key-Intermediate Methyl 1-Benzyl-5-methoxy-1H-indole-3-acetate and the Syntheses of Serotonin, Melatonin, and Bufotenin
AUTHOR(S): Revial, Gilbert; Jabin, Ivan; Lim, Sethy; Pfau, Michel
CORPORATE SOURCE: Laboratoire de Chimie Organique, CNRS (ESA 7084), ESPCI, Paris, 75231, Fr.
SOURCE: Journal of Organic Chemistry (2002), 67(7), 2252-2256
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:355101
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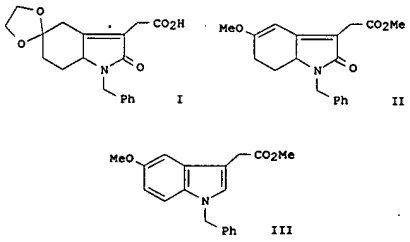
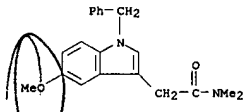


AB The imine of 1,4-cyclohexanedione mono-ethylene ketal was reacted with maleic anhydride, affording the cyclized adduct I. Me esterification of I, accompanied by transacetalization, led to the dihydrooxindole derivative II. Aromatization of II was then accomplished with POCl3, leading directly to the key-intermediate title compound III in 74% yield from the ketone. Serotonin, melatonin, and bufotenin were then obtained by standard reactions.
IT 419569-94-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(novel aromatization of tetrahydro-2H-indol-2-ones in the preparation of key-intermediate 1-benzyl-5-methoxy-1H-indole-3-acetate)
RN 419569-94-1 CAPLUS
CN 1H-Indole-3-acetamide, 5-methoxy-N,N-dimethyl-1-(phenylmethyl)- (9CI) (CA

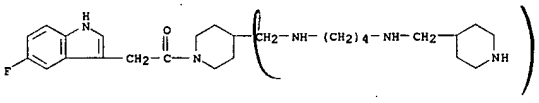
L3 ANSWER 16 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
INDEX NAME)



REFERENCE COUNT: 55 THERE ARE 55 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

R3 + R4 = subst. alkylene bridge

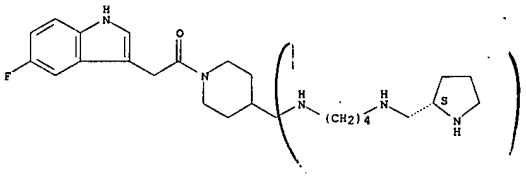
L3 ANSWER 17 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
receptor antagonists)
RN 396071-91-3 CAPLUS
CN 4-Piperidinemethanamine, 1-[(5-fluoro-1H-indol-3-yl)acetyl]-N-[4-[(4-piperidinylmethyl)amino]butyl]-, trihydrochloride (9CI) (CA INDEX NAME)



●3 HCl

RN 396071-92-4 CAPLUS
CN 4-Piperidinemethanamine, 1-[(5-fluoro-1H-indol-3-yl)acetyl]-N-[4-[[(2S)-2-pyrrolidinylmethyl]amino]butyl]-, trihydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

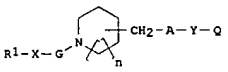


●3 HCl

L3 ANSWER 17 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:113840 CAPLUS
DOCUMENT NUMBER: 136:167283
TITLE: Preparation of acetylpiperidinebutanediamines as calcium ion-permeable AMPA receptor antagonists
INVENTOR(S): Mimura, Tetsuya; Kawajiri, Shinichi
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 93 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002047272	A	20020212	JP 2000-225300	20000726
PRIORITY APPLN. INFO.:			JP 2000-225300	20000726

OTHER SOURCE(S): MARPAT 136:167283
GI



I

AB The compds. I (R1 = aryl, arylcarbonyl, aryloxy, cycloalkyl heterocyclyl, etc.; X = single bond, (un)substituted alkyl, alkenyl, cycloalkyl, monocyclic heterocyclyl; G = CO, SO2; n = 0-3; A = NR2, O, S, single bond; R2 = H, alkyl, OH; Y = alkylene, alkynylene, alkenylene; Q = NR3R4, OR5, SR5; R3, R4 = H, alkyl, cycloalkyl, aralkyl, etc.; R5 = alkyl, cycloalkyl, aryl, heterocyclyl, etc.), their salts, and solvates are prepared The compds. are useful for cerebral infarction, senile dementia, Alzheimer's, disease, Parkinson's disease, and Huntington's disease. Cyclohexanol was reacted with with oxalyl chloride in the presence of DMSO and Et3N in CH2Cl2 at -78° for 30 min and reacted with 4-[N-(4-aminobutyl)-N-(tert-butoxycarbonyl)aminomethyl]-1-(1-naphthylacetyl)piperidine for 1 h to give 82% N-(tert-butoxycarbonyl)-N'-cyclohexylmethyl-N-[1-(1-naphthylacetyl)piperidin-4-ylmethyl]-1,4-butanediamine, which was treated with HCl in EtOH at room temperature for 5 h to give N-cyclohexylmethyl-N'-[1-(1-naphthylacetyl)piperidin-4-ylmethyl]-1,4-butanediamine hydrochloride showing good AMPA receptor blocking activity in vitro.
IT 396071-91-3P 396071-92-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acetylpiperidinebutanediamines as calcium ion-permeable AMPA

L3 ANSWER 18 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2002:6386 CAPLUS
DOCUMENT NUMBER: 136:69731
TITLE: Preparation of N-phenylthiophenecarboxamidines and analogs as NO synthase and lipid peroxidation inhibitors
INVENTOR(S): Chabrier de Lassauniere, Pierre Etienne; Auvin, Serge; Bigg, Dennis; Auguet, Michel; Harnett, Jeremiah
PATENT ASSIGNEE(S): Societe de Conseils de Recherches et d'Applications Scientifiques (S.C.R.A.S.), Fr.
SOURCE: U.S., 63 pp., Cont.-in-part of U. S. Ser. No. 381,749.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6335445	B1	20020101	US 1999-456205	19991207
FR 2761066	A1	19980925	FR 1997-3528	19970324
FR 2761066	B1	20001124		
FR 2764889	A1	19981224	FR 1997-7701	19970620
FR 2764889	B1	20000901		
WO 9842696	A1	19981001	WO 1998-FR288	19980216
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 6340700	B1	20020122	US 1999-381749	19990922
US 2002007062	A1	20020117	US 2001-882264	20010615
US 6630461	B2	20031007		
US 2002045753	A1	20020418	US 2001-945782	20010904
US 6599903	B2	20030729		
US 2002042511	A1	20020411	US 2001-953682	20010917
US 6586454	B2	20030701		
US 2003078420	A1	20030424	US 2002-191950	20020709
US 6809088	B2	20041026		
US 2005043397	A1	20050224	US 2004-898916	20040726
US 7122535	B2	20061017		
US 2005187272	A1	20050825	US 2005-105291	20050413

PRIORITY APPLN. INFO.:

FR 1997-3528	A	19970324
FR 1997-7701	A	19970620
WO 1998-FR288	W	19980216
US 1999-381749	A2	19990922
WO 1998-FR1250	W	19980615
US 1999-456205	A3	19991207
US 2001-882264	A3	20010615

L3 ANSWER 18 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
US 2002-191950 A3 20020709

US 2004-898916 A3 20040726

OTHER SOURCE(S): MARPAT 136:69731
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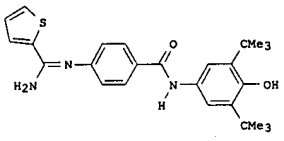
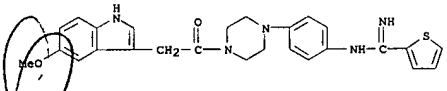


II

AB RZZ1Z2Z3N:C(NH2)R1 [I; R = H, (un)substituted C6H4OR3, indolyl, etc.; R1 = alkyl or (un)substituted (hetero)aryl; R3 = H, alkyl, etc.; Z = bond, CO, alkylene(carbonyl), CONH, etc.; Z1 = bond or heterocyclylene; Z2 = bond, alkylene(oxy), etc.; Z3 = (un)substituted phenylene] were prepared Thus, 4-(O2N)C6H4NH2 was amidated by 3,5-di-tert-butyl-4-hydroxybenzoic acid and the reduced product amidated by S-methyl-2-thiophenethiocarboximide hydroiodide to give title compound II. Data for biol. activity of I were given.

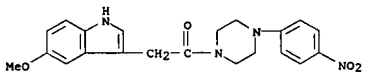
IT 214123-85-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-phenylthiophenecarboxamidines and analogs as NO synthase and lipid peroxidn. inhibitors)

RN 214123-85-0 CAPLUS
CN Piperazine, 1-[4-[(imino-2-thienylmethyl)amino]phenyl]-4-[(5-methoxy-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)

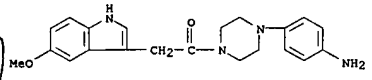


IT 214124-59-1P 214124-60-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-phenylthiophenecarboxamidines and analogs as NO synthase and lipid peroxidn. inhibitors)

L3 ANSWER 18 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 214124-59-1 CAPLUS
CN Piperazine, 1-[(5-methoxy-1H-indol-3-yl)acetyl]-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 214124-60-4 CAPLUS
CN Piperazine, 1-(4-aminophenyl)-4-[(5-methoxy-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:868447 CAPLUS
DOCUMENT NUMBER: 136:5917
TITLE: Preparation of (hetero)arylacyl-piperidinyl-benzylamines for use as tryptase inhibitors
INVENTOR(S): Astles, Peter C.; Eastwood, Paul R.; Houille, Olivier; Levell, Julian; Pauls, Heinz; Czekaj, Mark; Liang, Guyan; Gong, Yong; Pribish, James; Neuenschwander, Kent
PATENT ASSIGNEE(S): Aventis Pharmaceuticals Products Inc., USA
SOURCE: PCT Int. Appl., 267 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001090101	A1	20011129	WO 2001-US13811	20010427
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2003187020	A1	20031002	US 2001-843126	20010426
US 6977263	B2	20051220		
CA 2409827	A1	20011129	CA 2001-2409827	20010427
EP 1296972	A1	20030402	EP 2001-930925	20010427
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ZA 2002009484	A	20040223	ZA 2002-9484	20021121
HK 1057899	A1	20060728	HK 2004-100765	20040206
US 2005228018	A1	20051013	US 2005-57809	20050214
PRIORITY APPLN. INFO.:			GB 2000-12362 A	20000522
			US 2001-843126 A	20010426
			CN 2001-811952 A3	20010427
			WO 2001-US13811 W	20010427

OTHER SOURCE(S): MARPAT 136:5917
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

L3 ANSWER 19 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

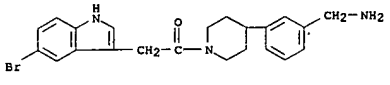
AB Title compds. I [Ar = (hetero)aryl, where the two groups on the Ar ring are β to each other; R1-2 = H, alkyl; R3 = (un)substituted(hetero)aryl, arylalkenyl, cycloalkenyl, cycloalkyl, etc.; R4 = H, acyl, alkoxy, alkyloxycarbonyl, carboxy, CN, halo, etc.; n = 0 - 4] were prepared Over 300 synthetic examples were disclosed. For instance, 3-bromobenzylbromide was converted in two steps to boronate II. II was coupled to the triflate ester derivative of the enol of 4-oxo-N-benzyloxycarbonylpiperidine (DMF, K2CO3, PdCl2(dppf)•CH2Cl2, 80°C, 18 h) to give the corresponding bicyclic intermediate. This intermediate was deprotected and reduced to the piperidine (EtOH, 10% Pd-C/H2, room temperature, 5 h) and coupled to 5-phenethylthiophene-2-carboxylic acid (DMF, HAPyU, iPr2NEt, room temperature, 18 h) to give III. III had Ki = 50 nM for tryptase. I are useful in the treatment of e.g., asthma and inflammatory diseases.

IT 375851-79-9P
RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug; preparation of (hetero)arylacyl-piperidinyl-benzylamines for use as tryptase inhibitors)

RN 375851-79-9 CAPLUS
CN Piperidine, 4-[3-(aminomethyl)phenyl]-1-[(5-bromo-1H-indol-3-yl)acetyl]-, trifluoroacetate (9CI) (CA INDEX NAME)

CM 1

CRN 375851-78-8
CMF C22 H24 Br N3 O



CM 2

CRN 76-05-1
CMF C2 H F3 O2

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L3 ANSWER 20 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

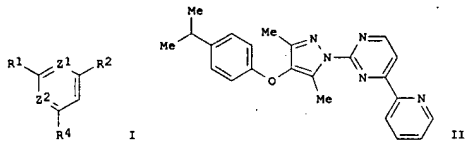
ACCESSION NUMBER: 2001:851126 CAPLUS
DOCUMENT NUMBER: 135:371760
TITLE: Preparation of pyrazolylpyrimidines and analogs as TNF-α signaling modulators
INVENTOR(S): Sneddon, Scott F.; Kane, John L.; Hirth, Bradford H.; Vinick, Fred; Qiao, Shuang; Nahill, Sharon R.
PATENT ASSIGNEE(S): Genzyme Corporation, USA
SOURCE: PCT Int. Appl., 108 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001087849	A2	20011122	WO 2001-US15027	20010510
WO 2001087849	A3	20020606		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2408408	A1	20011122	CA 2001-2408408	20010510
US 2002119988	A1	20020829	US 2001-852965	20010510
US 6969728	B2	20051129		
EP 1294699	A2	20030326	EP 2001-933253	20010510
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003533515	T	20031111	JP 2001-584245	20010510
BR 2001011158	A	20040406	BR 2001-11158	20010510
NO 2002005405	A	20030109	NO 2002-5405	20021111
US 2004171617	A1	20040902	US 2004-797244	20040310
US 7034031	B2	20060425		
US 2006173010	A1	20060803	US 2005-292325	20051201

PRIORITY APPLN. INFO.:	US 2000-203784P	P	20000512
	US 2000-205213P	P	20000518
	US 2001-852965	A3	20010510
	WO 2001-US15027	W	20010510
	US 2004-797244	A1	20040310

OTHER SOURCE(S): MARPAT 135:371760
GI

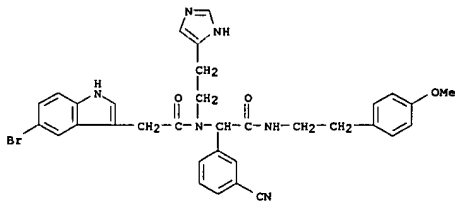
L3 ANSWER 20 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB Title compds. [I; R1 = H or NH2; R2 = ZZ3(CH2)nR; R = (un)substituted Ph or -heterocyclyl; R4 = (alkyl-substituted) 2-pyridinyl or -pyrazinyl; Z = (un)substituted pyrazole-1,4-diyl; Z1,Z2 = N or CH; Z3 = O, CH2, S, SO2; n = 0-2] were prepared Thus, 4-(Me2HC)C6H4OH was condensed with (MeCO)2CHN2 and the product cyclocondensed with 4-(2-pyridinyl)-2-pyrimidinylhydrazine to give title compound II. Data for biol. activity of I were given.

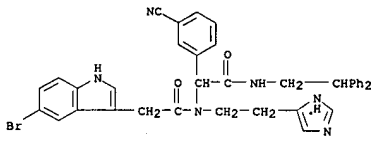
IT 374080-55-4P 374080-62-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolylpyrimidines and analogs as TNF-α signaling modulators)

RN 374080-55-4 CAPLUS
CN 1H-Indole-3-acetamide, 5-bromo-N-[1-(3-cyanophenyl)-2-[[2-(4-methoxyphenyl)ethyl]amino]-2-oxoethyl]-N-[2-(1H-imidazol-4-yl)ethyl]- (9CI) (CA INDEX NAME)



RN 374080-62-3 CAPLUS
CN 1H-Indole-3-acetamide, 5-bromo-N-[1-(3-cyanophenyl)-2-[(2,2-diphenylethyl)amino]-2-oxoethyl]-N-[2-(1H-imidazol-4-yl)ethyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 20 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



R^3 + Cy = 5 or 6 alkyl

L3 ANSWER 21 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:762989 CAPLUS
DOCUMENT NUMBER: 135:318419
TITLE: Synthesis of substituted bipiperidines and their use as H1 antagonists
INVENTOR(S): Lawrence, Louise; Rigby, Aaron; Sanganee, Hitesh; Springthorpe, Brian
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 160 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

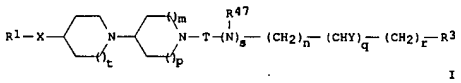
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001077101	A1	20011018	WO 2001-SE751	20010405
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2403012	A1	20011018	CA 2001-2403012	20010405
EP 1274701	A1	20030115	EP 2001-920053	20010405
EP 1274701	B1	20050629		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001009922	A	20030218	BR 2001-9922	20010405
CN 1433411	A	20030730	CN 2001-810683	20010405
JP 2003530393	T	20031014	JP 2001-575574	20010405
NZ 521543	A	20041029	NZ 2001-521543	20010405
EP 1493743	A1	20050105	EP 2004-20599	20010405
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, CY, TR				
AT 298748	T	20050715	AT 2001-920053	20010405
CN 1660839	A	20050831	CN 2004-10102245	20010405
US 2002077337	A1	20020620	US 2001-827488	20010406
US 6525070	B2	20030225		
ZA 2002007700	A	20040102	ZA 2002-7700	20020925
NO 2002004774	A	20021129	NO 2002-4774	20021003
US 2004006080	A1	20040108	US 2003-341027	20030113
US 6903115	B2	20050607		
US 2004014783	A1	20040122	US 2003-436582	20030513
HK 1051193	A1	20051028	HK 2003-103424	20030514
US 2005171092	A1	20050804	US 2005-76773	20050310

PRIORITY APPLN. INFO.: GB 2000-8626 A 20000408
GB 2000-19111 A 20000803
SE 2000-3664 A 20001011

L3 ANSWER 21 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

			CN 2001-810683	A3 20010405
			EP 2001-920053	A3 20010405
			WO 2001-SE751	W 20010405
			US 2001-827488	A3 20010406
			US 2003-341027	A1 20030113
			US 2003-436582	A3 20030513

OTHER SOURCE(S): MARPAT 135:318419
GI



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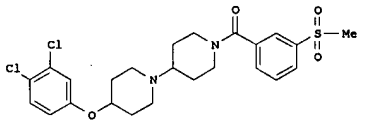
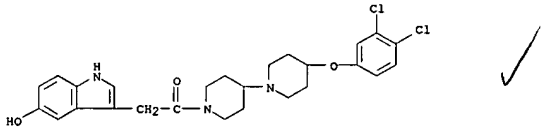


II

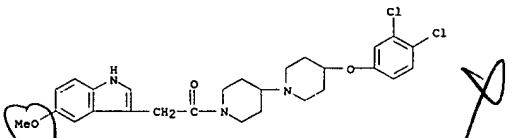
AB Title compds. I [q, s, t = 0 - 1; n, r = 0 - 5; m, p = 0 - 2; X = CH, C(O), O, S, S(O), S(O), N-; provided that when m and p are both 1 then X is not CH; Y = NHR2, OH; T = C(O), C(S), S(O), CH2; R1 = H, alkyl, aryl, heterocyclyl; R2, R47 = H, alkyl, aryl-alkyl, CO-alkyl; R3 = alkyl, alkenyl, cycloalkyl, cycloalkenyl, aryl, heterocyclyl, thioaryl, thioheterocyclyl] were prepared Examples include: data for over 600 compds., 4 solid oral dosage and 1 parenteral (general) formulations, a bioassay for Ca2+ flux, human eosinophil chemotaxis and H1 antagonism. E.g., 4-(3,4-dichlorophenoxy)piperidine was alkylated with 1-(tert-butoxycarbonyl)-4-piperidone (1,2-dichloroethane, NaBH(OAc)3, HOAc, 18 h, room temperature) to give an intermediate [1,4']bipiperidine. This intermediate was deprotected (DCM, TFA, 4 h, room temperature) and the resulting bipiperidine condensed with 3-methanesulfonylbenzoic acid (THF, PYBROP, (i-Pr)2NEt, 18 h, room temp.) to give example compd. II isolated as the acetate salt. I are used in the treatment of a chemokine (such as CCR3) or H1 mediated disease state.

IT 367497-01-6P 367498-68-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug; synthesis of substituted bipiperidines and use as H1 antagonists)

RN 367497-01-6 CAPLUS
CN 1,4'-Bipiperidine, 4-(3,4-dichlorophenoxy)-1'-[(5-hydroxy-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)



RN 367498-68-8 CAPLUS
CN 1,4'-Bipiperidine, 4-(3,4-dichlorophenoxy)-1'-[(5-methoxy-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

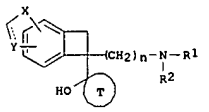
L3 ANSWER 22 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:760046 CAPLUS
DOCUMENT NUMBER: 135:303899
TITLE: Synthesis of heterocycloalkylbenzocyclobutanes and heteroarylbenzocyclobutanes and their use as inhibitors of serotonin and noradrenaline reuptake
INVENTOR(S): Peglion, Jean-Louis; Dessinges, Aimee; Goument, Bertrand; Millan, Mark; Lejeune, Francoise; Brocco, Mauricette
PATENT ASSIGNEE(S): Adir Et Compagnie, Fr.; Servier Lab
SOURCE: Eur. Pat. Appl., 47 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1146041	A1	20011017	EP 2001-400940	20010412
EP 1146041	B1	20031112		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
FR 2807753	A1	20011019	FR 2000-4742	20000413
FR 2807753	B1	20020607		
JP 2001302599	A	20011031	JP 2001-111169	20010410
JP 3761796	B2	20060329		
NO 2001001862	A	20011015	NO 2001-1862	20010411
NO 318158	B1	20050207		
BR 2001001444	A	20011204	BR 2001-1444	20010411
ZA 2001003065	A	20011018	ZA 2001-3065	20010412
US 2002019380	A1	20020214	US 2001-833827	20010412
US 6420413	B2	20020716		
HU 200101503	A2	20020529	HU 2001-1503	20010412
NZ 511092	A	20021025	NZ 2001-511092	20010412
AT 254102	T	20031115	AT 2001-400940	20010412
PT 1146041	T	20040331	PT 2001-400940	20010412
ES 2210104	T3	20040701	ES 2001-1400940	20010412
AU 777825	B2	20041104	AU 2001-35187	20010412
CN 1323794	A	20011128	CN 2001-116386	20010413
CA 2344255	A1	20011013	CA 2001-2344255	20010417
CA 2344255	C	20060711		
HK 1042477	A1	20050506	HK 2002-102196	20020322

PRIORITY APPLN. INFO.: FR 2000-4742 A 20000413

OTHER SOURCE(S): MARPAT 135:303899
GI

L3 ANSWER 22 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



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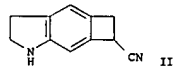
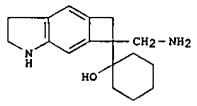


II



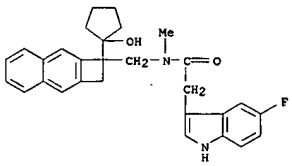
III

AB Title compds. I [n = 1 - 6; R1-2 = H, alkyl, aryl, arylalkyl, cycloalkyl(alkyl), alkenyl, alkynyl, heterocyclyl, etc.; X = CH:CH, O, SO0-2, NR3; Y = CH/CH2; T = cycloalkyl (mono or polycyclic), heterocyclyl] were prepared Forty example compds. were disclosed. E.g., 6-cyano-1-methylsulfonyl-5,6-dihydrocyclobuta[f]indole (preparation given) was desulfonylated (K, MeOH, reflux, 12 h) and converted to tetrahydro derivative II (HOAc, NaCNBH3, room temperature, 2 h). II was alkylated with cyclohexanone (THF, n-BuLi, -80°C) and the resulting nitrile reduced to aminomethyl derivative III (MeOH, H2-Ra/Ni, 30 bar, 60°C, 24 h). In competitive binding assays, compds. of the invention showed affinity for serotonin reuptake binding sites, pKi > 7 and noradrenaline reuptake binding sites, pKi ≥ 6. I are used to treat depression, panic attacks, anxiety, obesity, etc.

IT 367263-60-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; synthesis of heterocycloalkylbenzocyclobutanes and heteroarylbenzocyclobutanes and their use as inhibitors of serotonin and noradrenaline reuptake)

RN 367263-60-3 CAPLUS
CN 1H-Indole-3-acetamide, N-[[1,2-dihydro-1-(1-hydroxycyclopentyl)cyclobuta[b]naphthalen-1-yl]methyl]-5-fluoro-N-methyl- (9CI) (CA INDEX NAME)

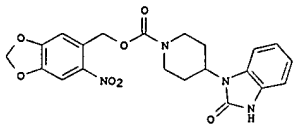
L3 ANSWER 22 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 23 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:667283 CAPLUS
DOCUMENT NUMBER: 136:179
TITLE: From Hit to Lead. Combining Two Complementary Methods for Focused Library Design. Application to μ Opiate Ligands
AUTHOR(S): Poulain, Rebecca; Horvath, Dragos; Bonnet, Beatrice; Eckhoff, Christian; Chapelain, Beatrice; Bodinier, Marie-Christine; Deprez, Benoit
CORPORATE SOURCE: Department of Chemistry, CEREP, Lille, F-59000, Fr.
SOURCE: Journal of Medicinal Chemistry (2001), 44(21), 3378-3390
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 136:179
GI



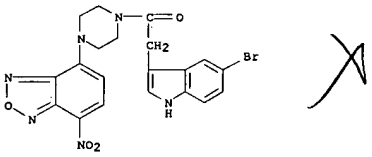
I

AB Compound I obtained by random screening and displaying a micromolar activity on the μ opiate receptor was chosen as a starting point for optimization. Two complementary concepts of similarity were used for the design of analogs and compared. These are based, resp., on a computer-aided comparison of pharmacophoric patterns and on topol. similarity. The structure-activity relationships are discussed in light of both similarity concepts. An N-methyl-3-(4-oxo-1-phenyl-1,3,8-triazaspiro[4.5]decyl)acetamide derivative, designed by combining the structure-activity relationships enlightened by each method, has a subnanomolar affinity for μ (h) receptor (IC50 = 0.9 nM). It is a promising lead, allowing the design of a new series of analogs substituted at the N-3 of the spirocycle moiety.

IT 372956-13-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(combining two complementary methods for focused library design and application to μ opiate ligands)

RN 372956-13-3 CAPLUS
CN Piperazine, 1-[(5-bromo-1H-indol-3-yl)acetyl]-4-(7-nitro-2,1,3-benzoxadiazol-4-yl)- (9CI) (CA INDEX NAME)

L3 ANSWER 23 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



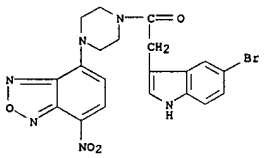
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 24 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:662562 CAPLUS
DOCUMENT NUMBER: 135:352346
TITLE: From Hit to Lead. Analyzing Structure-Profile Relationships
AUTHOR(S): Poulain, Rebecca; Horvath, Dragos; Bonnet, Beatrice; Eckhoff, Christian; Chapelain, Beatrice; Bodinier, Marie-Christine; Deprez, Benoit
CORPORATE SOURCE: Department of Chemistry, CEREP, Lille, F-59000, Fr.
SOURCE: Journal of Medicinal Chemistry (2001), 44(21), 3391-3401
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two compds., (piperidine and piperazine carboxylic acid derivs.) obtained by random screening, and displaying micromolar activities on the μ opiate receptor were used as starting points for optimization. In that work, the traditional concept of the activity of a compound (related to one or a few targets) was extended to the comprehensive pharmacol. profile of that compound on more than 70 receptors, transporters, and channels relevant to a CNS-oriented project. Using the two complementary design strategies based on two similarity concepts described in the previous paper, we have obtained analogs with IC50 values ranging between 0.9 nM and a few micromolar on the μ receptor and displaying qual. different profiles. We discuss here, both on a case-by-case basis and from a statistical standpoint, the pharmacol. profiles in light of the two similarity concepts.

IT 372956-13-3
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(piperidine- and piperazine carboxylic acid derivative opioid receptor structure-activity relationship, and compound preparation)

RN 372956-13-3 CAPLUS
CN Piperazine, 1-[(5-bromo-1H-indol-3-yl)acetyl]-4-(7-nitro-2,1,3-benzoxadiazol-4-yl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS

L3 ANSWER 24 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 25 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:565002 CAPLUS
DOCUMENT NUMBER: 135:152713
TITLE: Aromatic amides as novel melanocortin receptor agonists and antagonists
INVENTOR(S): Lundstedt, Torbjoern; Skottner, Anna; Seifert, Elisabeth; Starchenkov, Igor; Trapencieris, Peteris; Kauss, Valerjans; Kalvins, Ivars; Boman, Arne
PATENT ASSIGNEE(S): Melacure Therapeutics AB, Swed.
SOURCE: PCT Int. Appl., 52 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001055106	A2	20010802	WO 2001-GB346	20010129
WO 2001055106	A3	20020321		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2398728	A1	20010802	CA 2001-2398728	20010129
BR 2001007893	A	20021105	BR 2001-7893	20010129
EP 1254114	A2	20021106	EP 2001-946850	20010129
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003520850	T	20030708	JP 2001-555048	20010129
ZA 2002005886	A	20040621	ZA 2002-5886	20020723
US 2003195212	A1	20031016	US 2002-182192	20021120

PRIORITY APPLN. INFO.: GB 2000-1948 A 20000128
GB 2000-2060 A 20000128
WO 2001-GB346 W 20010129

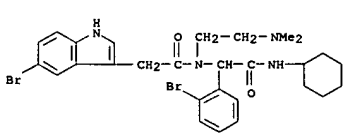
OTHER SOURCE(S): MARPAT 135:152713

AB The present invention relates to novel aromatic amides (I; B-E-X-N(R8)-C(O)-Y-F-A and pharmacol. active salts thereof) and to the use of these amides for the treatment of obesity, anorexia, inflammation, mental disorders and other diseases associated with the melanocortin receptors or related systems, e.g. the melanocyte stimulating hormones. In I: E and F are independently a saturated or unsatd., acyclic hydrocarbon group having 1-5 C atoms. X and Y are independently methylene; one of X and Y are absent (i.e. a single bond); or X can be -CH(QR10)- and/or Y can be -CH(MR9)- (M and Q are independently a saturated or unsatd., straight or branched chain acyclic hydrocarbon group with 1-6 C atoms; or M and/or Q are absent (i.e. M and/or Q are single bonds)). R8, R9 and R10 are H, -PR4, -C(O)DR4 (P and D are independently a saturated or unsatd., straight or

L3 ANSWER 25 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
branched chain acyclic hydrocarbon group having 1-6 C atoms; or D is absent (i.e. D is a single bond)). R4 is hydroxy, Me, cyclohexyl, cyclopentyl, aminoguanidine, guanidine, carboxy, or (possibly substituted) amino, carbamoyl, alkoxy, alkoxycarbonyl, acyl, morpholinyl, pyrrolidinyl, piperidinyl, piperazinyl, Ph, isoindolyl, indenyl, pyridinyl, indolyl, pyrrolyl, cyclopentadienyl wherein R4 in R8, R9 and R10 may be the same or different. A and B are the same or different and are (possibly substituted) quinolinyl, isoquinolinyl, isoindolyl, naphthyl, pyridinyl, indolyl, pyrazinyl, cyclopentadienyl, pyrimidinyl, Ph, indenyl. Several claimed compds. (N-(3-aminopropyl)-3-(1H-indol-3-yl)-2-(2-naphthalen-1-ylacetylamino)propionamide hydrochloride (1:1.2), N-[1-[benzyl(4-guanidinobutyl)carbamoyl]-2-(1H-indol-3-yl)ethyl]-4-phenylbutyramide monohydrochloride, N-benzyl-N-(4-guanidinobutyl)-3-(1H-indol-3-yl)-2-(2-naphthalen-2-ylacetylamino)propionamide monohydrochloride, N-[1-(9-ethyl-9H-carbazol-3-ylcarbamoyl)-2-(1H-indol-3-yl)ethyl]-4-guanidinobutyramide monohydrochloride, 4-amino-N-[1-(9-ethyl-9H-carbazol-3-ylcarbamoyl)-2-(1H-indol-3-yl)ethyl]butyramide monohydrochloride, 2-(3-aminopropionylamino)-N-(9-ethyl-9H-carbazol-3-yl)-3-(1H-indol-3-yl)propionamide monohydrochloride) were tested (results given) for affinity for melanocortin receptors (MC1, MC3, MC4, MC5) and/or influence on cAMP. In vivo effects on food intake and anti-inflammatory effects were also detd. on selected compds. Two example prepns. are given.

IT 352277-28-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(aromatic amides as novel melanocortin receptor agonists and antagonists and their preparation)

RN 352277-28-2 CAPLUS
CN 1H-Indole-3-acetamide, 5-bromo-N-[1-(2-bromophenyl)-2-(cyclohexylamino)-2-oxoethyl]-N-[2-(dimethylamino)ethyl]-, monohydrochloride (9CI) (CA INDEX NAME)



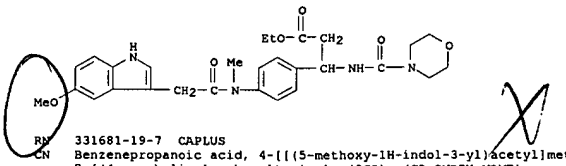
● HCl

L3 ANSWER 26 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:237851 CAPLUS
DOCUMENT NUMBER: 134:252261
TITLE: Preparation of heterocyclylcarbonylamino-modified phenylpropanes and their use as integrin VLA-4 binding inhibitors
INVENTOR(S): Yokota, Masaki; Nagashima, Shinya; Sugane, Takashi; Igarashi, Susumu; Moridaira, Koichiro; Miura, Ayanori; Ikeda, Masaru; Takeuchi, Makoto
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 20 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

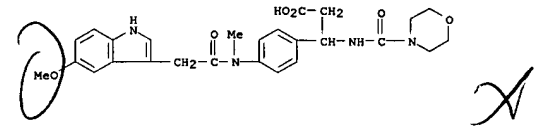
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001089448	A	20010403	JP 1999-271096	19990924
PRIORITY APPLN. INFO.:			JP 1999-271096	19990924

OTHER SOURCE(S): MARPAT 134:252261
AB 4-RcCH2CONRdC6H4CH(NReCORb)CH2CO2Ra [Ra = H, ester residue (prodrug); Rb = morpholino, 2,4-dioxo-1,2,3,4-tetrahydropyrimidin-5-yl; Rc = (un)substituted (hetero)aryl; Rd, Re = H, lower alkyl], useful for treatment of asthma, allergy, rheumatoid arthritis, autoimmune disease, rejection, inflammation, arteriosclerosis, cancer metastasis, diabetes, etc., are prepared Thus, a solution of 5-methoxyindoleacetic acid and Et (RS)-3-(4-aminophenyl)-3-[(morpholine-4-carbonyl)amino]propanoate in DMF was treated with WSC.HCl and HOBt at room temperature for 20 h to give the corresponding amide.
IT 331681-06-2P 331681-19-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclylcarbonylamino-modified phenylpropanes as integrin VLA-4 binding inhibitors for treatment of diseases)
RN 331681-06-2 CAPLUS
CN Benzenepropanoic acid, 4-[[(5-methoxy-1H-indol-3-yl)acetyl]methylamino]-β-[(4-morpholinylcarbonyl)amino]-, ethyl ester (9CI) (CA INDEX NAME)

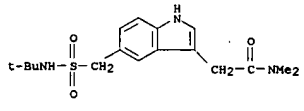
L3 ANSWER 26 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 331681-19-7 CAPLUS
CN Benzenepropanoic acid, 4-[[(5-methoxy-1H-indol-3-yl)acetyl]methylamino]-β-[(4-morpholinylcarbonyl)amino]- (9CI) (CA INDEX NAME)

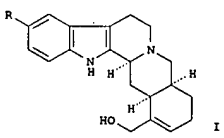


L3 ANSWER 27 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:83714 CAPLUS
DOCUMENT NUMBER: 134:311061
TITLE: Synthesis of 5-(sulfamoylmethyl)indoles
AUTHOR(S): Bosch, J.; Roca, T.; Armengol, M.; Fernandez-Forner, D.
CORPORATE SOURCE: Laboratory of Organic Chemistry, Faculty of Pharmacy, University of Barcelona, Barcelona, 08028, Spain
SOURCE: Tetrahedron (2001), 57(6), 1041-1048
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:311061
AB The synthesis of 5-(sulfamoylmethyl)indoles bearing a two-carbon chain at C-3 (aminoethyl, acetate, hydroxyethyl, ethyl) either by the Grandberg modification of the Fischer indolization or by intramol. Heck reaction of suitable o-halotrifluoroacetanilides is reported.
IT 334981-21-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 5-(sulfamoylmethyl)indoles)
RN 334981-21-4 CAPLUS
CN 1H-Indole-3-acetamide, 5-[[[(1,1-dimethylethyl)amino]sulfonyl]methyl]-N,N-dimethyl- (9CI) (CA INDEX NAME)



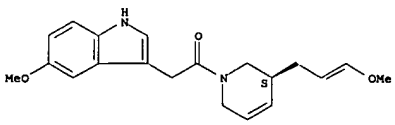
REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 28 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2001:77719 CAPLUS
DOCUMENT NUMBER: 134:222897
TITLE: Cascading single-step stereoselective construction of the α-alloyohimbine framework: a new synthesis of (-)-nitraraine
AUTHOR(S): Sakagami, Hideki; Ogasawara, Kunio
CORPORATE SOURCE: Pharmaceutical Institute, Tohoku University, Sendai, 980-8578, Japan
SOURCE: Heterocycles (2001), 54(1), 43-47
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:222897
GI



AB (-)-Nitraraine (I, R = H) and its 10-methoxy analog (I, R = OMe) having an α-alloyohimbine framework have been constructed stereoselectively in a cascading single step sequence from chiral mono-substituted N-2-(3-indolyl)ethyltetrahydropyridine precursors under the Heck reaction conditions.
IT 329771-40-6P 329771-41-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of (-)-nitraraine via a cascading single-step stereoselective construction of the α-alloyohimbine framework)
RN 329771-40-6 CAPLUS
CN Pyridine, 1,2,3,6-tetrahydro-1-[(5-methoxy-1H-indol-3-yl)acetyl]-3-(3-methoxy-2-propenyl)-, (3S)- (9CI) (CA INDEX NAME)

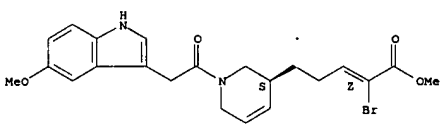
Absolute stereochemistry.
Double bond geometry unknown.



RN 329771-41-7 CAPLUS
CN 2-Pentenoic acid, 2-bromo-5-[(3S)-1,2,3,6-tetrahydro-1-[(5-methoxy-1H-

L3 ANSWER 28 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
indol-3-yl)acetyl]-3-pyridinyl]-, methyl ester, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

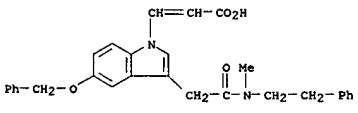
L3 ANSWER 29 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:772622 CAPLUS
DOCUMENT NUMBER: 133:335167
TITLE: Preparation of diaryl carboxylic acids and derivatives
as peroxisome proliferator-activated receptor ligands.
INVENTOR(S): Jayyosi, Zaid; McGeehan, Gerard M.; Kelley, Michael F.; Labaudiniere, Richard F.; Zhang, Litao; Groneberg,
Robert D.; McGarry, Daniel G.; Caulfield, Thomas J.; Minnich, Anne; Bobko, Mark
PATENT ASSIGNEE(S): Aventis Pharmaceuticals Products Inc., USA
SOURCE: PCT Int. Appl., 167 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000064888	A1	20001102	WO 2000-US11833	20000428
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2370250	A1	20001102	CA 2000-2370250	20000428
EP 1177187	A1	20020206	EP 2000-928698	20000428
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
BR 2000010605	A	20020213	BR 2000-10605	20000428
HU 200201291	A2	20020928	HU 2002-1291	20000428
EE 200100556	A	20030217	EE 2001-556	20000428
NZ 515086	A	20031031	NZ 2000-515086	20000428
AU 781266	B2	20050512	AU 2000-46895	20000428
RU 2267484	C2	20060110	RU 2001-132080	20000428
US 6635655	B1	20031021	US 2000-662649	20000914
NO 2001005075	A	20011123	NO 2001-5075	20011018
ZA 2001008798	A	20030305	ZA 2001-8798	20011024
HR 2001000795	A1	20030228	HR 2001-795	20011026

PRIORITY APPLN. INFO.: US 1999-131455P P 19990428
WO 2000-US11833 W 20000428

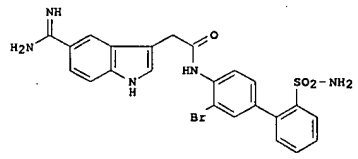
OTHER SOURCE(S): MARPAT 133:335167
AB Ar1(CR1R2)aA(CR3R4)bAr2(CR5R6)cB(CR7R8)dE{Ar1, Ar2 = aryl, fused arylcycloalkenyl, fused arylcycloalkyl, fused arylheterocycloalkenyl, fused arylheterocyclyl, heteroaryl, fused heteroarylcycloalkenyl, fused heteroarylcycloalkyl, fused heteroarylheterocyclyl, etc.; A = O, S, SO, SO2, NR13, CO, NR14CO, CONR15, NR14CONR15, CR14:N, bond, etc.; B = O, S, NR19, bond, CO, NR20CO, CONR20; E = bond, CH2CH2; Z = R21O2C, R21OC,

L3 ANSWER 29 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
cycloimide, cyano, R21O2SHNCO, R21O2SHN, (R21)2NCO, R21O-substituted 2,4-thiazolidinedionyl, tetrazolyl; a, d = 0-6; b, c = 0-4; R1, R3, R5, R7
= H, halo, alkyl, CO2H, alkoxycarbonyl, aralkyl; R2, R4, R6, R8 = (CH2)qX;
q = 0-3; R14, R15, R20 = H, alkyl, aralkyl, CO, alkoxycarbonyl; R14R15 = atoms to form a 5-6 membered azaheterocyclyl; R19, R21 = H, aryl, alkyl, cycloalkyl, aralkyl], were prepd. as agonists or antagonists of the PPAR receptor (no data). Thus, 3-(quinolin-2-ylmethoxy)propan-1-ol in DMPU/THF
at 0° was treated with NaH and then with Me 2-bromomethyl-6-methylbenzoate followed by stirring overnight at room temp. to give Me 2-methyl-6-[3-(quinolin-2-ylmethoxy)propoxymethyl]benzoate.
IT 141835-21-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diaryl carboxylic acids and derivs. as PPAR ligands)
RN 141835-21-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[2-[methyl(2-phenylethyl)amino]-2-oxoethyl]-5-(phenylmethoxy)-1H-indol-1-yl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

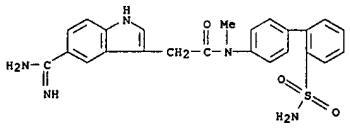
L3 ANSWER 30 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:762637 CAPLUS
DOCUMENT NUMBER: 134:86116
TITLE: Design, Synthesis, and Biological Evaluation of Potent
and Selective Amidino Bicyclic Factor Xa Inhibitors
AUTHOR(S): Han, Qi; Dominguez, Celia; Stouten, Pieter F. W.; Park, Jeongsook M.; Duffy, Daniel E.; Galemmo, Robert A., Jr.; Rossi, Karen A.; Alexander, Richard S.; Smallwood, Angela M.; Wong, Pancras C.; Wright, Matthew M.; Leuttgen, Joseph M.; Knabb, Robert M.; Wexler, Ruth R.
CORPORATE SOURCE: DuPont Pharmaceuticals Company, Wilmington, DE, 19880-0500, USA
SOURCE: Journal of Medicinal Chemistry (2000), 43(23), 4398-4415
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 134:86116
GI



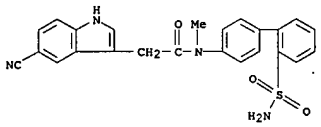
I

AB A novel series of factor Xa (fXa) inhibitors incorporating an amidino 6,5-fused bicyclic moiety, e.g. I (R = Me, F, Cl, Br, etc.), has been designed and synthesized based on mol. modeling studies. Structure-activity relationship (SAR) studies have led to selective subnanomolar fXa inhibitors. The most potent fXa inhibitor in this series
I (R = Br) has a potent inhibition constant (Ki = 0.3 nM), is 350-fold selective for fXa over trypsin, and also shows good in vivo efficacy in a rabbit arterio-venous thrombosis model (ID50 = 0.14 μmol/kg/h). An X-ray crystal structure of I (R = Br) complexed to bovine trypsin was completed, and its binding mode with fXa has been proposed based on modeling with human des-Gla-fXa.
IT 202124-24-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation and antithrombotic activities of amidino bicyclic factor Xa
inhibitors)
RN 202124-24-1 CAPLUS
CN 1H-Indole-3-acetamide, 5-(aminoiminomethyl)-N-[2'-(aminosulfonyl)[1,1'-

L3 ANSWER 30 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
biphenyl]-4-yl]-N-methyl- (9CI) (CA INDEX NAME)

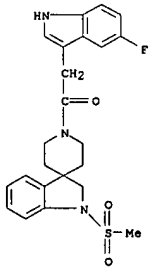


IT 316364-41-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and antithrombotic activities of amidino bicyclic factor Xa
inhibitors)
RN 316364-41-7 CAPLUS
CN 1H-Indole-3-acetamide,
N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-5-cyano-
N-methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 43 THERE ARE 43 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 31 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of spiro-substituted azacycles as neurokinin antagonists)
RN 167485-09-8 CAPLUS
CN Spiro[3H-indole-3,4'-piperidine],
1'-[(5-fluoro-1H-indol-3-yl)acetyl]-1,2-
dihydro-1-(methylsulfonyl)- (9CI) (CA INDEX NAME)

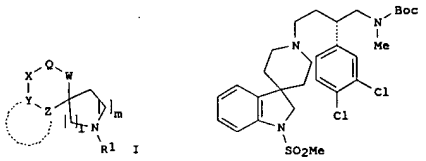


REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 31 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2000:31350 CAPLUS
DOCUMENT NUMBER: 132:78470
TITLE: Preparation of spiro-substituted azacycles as neurokinin antagonists
INVENTOR(S): Maccoss, Malcolm; Mills, Sander G.; Shah, Shrenik K.; Chiang, Yuan-ching P.; Dunn, Patrick T.; Koyama, Hiroo
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 49 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6013652	A	20000111	US 1997-985338	19971204
PRIORITY APPLN. INFO.:			US 1997-985338	19971204

OTHER SOURCE(S): MARPAT 132:78470
GI

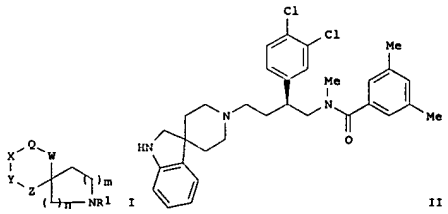


AB The title compds. [I; l, m = 0-5 (with the proviso that l + m = 1-5); R1 =
H, alkyl, alkenyl, etc.; W = a bond, (un)substituted alkyl; Q = O, S, SO, SO2, NR2 (with the proviso that when W = a bond and X = alkyl, then Q must
be NR2; R2 = H, alkyl, etc.); X = a bond, (un)substituted alkyl, NHCO, etc.; YZ considered together are 2 adjoining atoms of Ph, naphthyl, heteroaryl; the nitrogen in one of the rings is optionally quaternized with alkyl or phenylalkyl or is optionally present as an N-oxide], tachykinin receptor antagonists useful in the treatment of inflammatory diseases, pain or migraine, and asthma, were prepared E.g., a 2-step synthesis of 3-(S)-II was given. In particular compds. I are shown to be neurokinin antagonists, and, e.g., they have been found to displace radioactive ligand for the NK-1 receptor at 0.01 nM to 1.0 μM, for the NK-2 receptor , 0.01 nM to 5 μM, and for the NK-3 receptor, 1.0 nM to 10 μM.
IT 167485-09-8P

L3 ANSWER 32 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:635463 CAPLUS
DOCUMENT NUMBER: 131:243191
TITLE: Spiro-substituted azacycles as modulators of chemokine
receptor activity
INVENTOR(S): Mills, Sander G.; MacCoss, Malcolm; Springer, Martin S.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 97 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

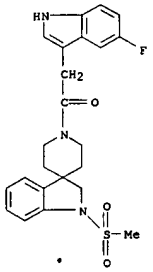
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 5962462	A	19991005	US 1997-989947		19971212
PRIORITY APPLN. INFO.:			US 1996-32735P	P	19961213
			US 1996-33558P	P	19961220

OTHER SOURCE(S): MARPAT 131:243191
GI



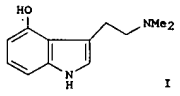
AB The invention is directed to spiro-substituted azacycles which are useful as modulators of chemokine receptor activity. Specifically, I [R1 = H, (un)substituted alk(en/yn)yl; W = bond, (un)substituted alkylene; Q = (un)substituted NH, O, S, S(O), SO2; X = bond, (un)substituted alkylene, S, S(O), NHCO, OC(O), etc.; YZ = fused aryl or heteroaryl nucleus; m, n = 0 to 5; (m+n) = 1 to 5] were prepared The compds. are useful as modulators
of the chemokine receptors CCR-1, CCR-2, CCR-2A, CCR-2B, CCR-3, CCR-4, CCR-5, CXCR-3, and/or CXCR-4 (no data), and are thereby useful as antiinflammatory and immunomodulating agents. Use for the treatment of HIV infection and/or AIDS is claimed specifically. For instance, 1'-methylspiro[indoline-3,4'-piperidine] underwent a sequence of N-benzoyloxycarbonylation (71%), N'-demethylation (73%), reductive

L3 ANSWER 32 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
N'-alkylation with a corresponding polyfunctional aldehyde, and removal of
the benzoyloxycarbonyl protecting group, to give title compd. II.
IT 167485-09-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
(target compound; preparation of spiro-substituted azacycles as modulators of
chemokine receptor activity)
RN 167485-09-8 CAPLUS
CN Spiro[3H-indole-3,4'-piperidine], 1'-[(5-fluoro-1H-indol-3-yl)acetyl]-1,2-dihydro-1-(methylsulfonyl)- (9CI) (CA INDEX NAME)



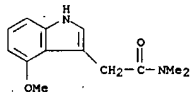
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 33 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:306450 CAPLUS
DOCUMENT NUMBER: 131:102423
TITLE: A new synthesis of psilocin
AUTHOR(S): Sakagami, Hideki; Ogasawara, Kunio
CORPORATE SOURCE: Pharmaceutical Institute, Tohoku University, Sendai, 980-8578, Japan
SOURCE: Heterocycles (1999), 51(5), 1131-1135
CODEN: HTCYAM; ISSN: 0385-5414
PUBLISHER: Japan Institute of Heterocyclic Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:102423
GI



I

AB A new route to the hallucinogenic alkaloid psilocin (I), isolated from the mushroom species Psilocybe mexicana, has been established.
IT 52335-79-2P, N,N-Dimethyl-4-methoxyindole-3-acetamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(new synthesis of psilocin from methoxy aniline dimethoxydihydrofuran)
RN 52335-79-2 CAPLUS
CN 1H-Indole-3-acetamide, 4-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

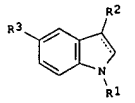


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 34 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1999:205361 CAPLUS
DOCUMENT NUMBER: 130:252241
TITLE: Preparation of amidinoindoles and analogs as factor Xa inhibitors
INVENTOR(S): Dominguez, Celia; Han, Qi; Duffy, Daniel Emmett; Park, Jeongsook Maria; Quan, Mimi Lifen; Rossi, Karen Anita; Wexler, Ruth Richmond
PATENT ASSIGNEE(S): Dupont Pharmaceuticals Company, USA
SOURCE: U.S., 46 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5886191	A	19990323	US 1997-916736	19970818
US 6043257	A	20000328	US 1998-176037	19981021
PRIORITY APPLN. INFO.:			US 1997-916736	A3 19970818

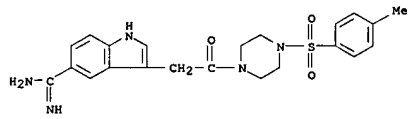
OTHER SOURCE(S): MARPAT 130:252241
GI



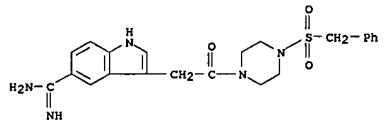
I

AB Title compds., e.g., I [R1 = H or Me; R2 = (CH2)nZZ1R; R = C(:NH)NH2, CH2Ph, C6H4(SO2NHR4)-2, etc.; R3 = C(:NH)NH2, cyano, etc.; R4 = alkyl; Z = CO, CONH, etc.; Z1 = C6H4, CH2C6H4, pyridine-2,4-diyl, etc.; n = 0 or 1; dashed line = optional addnl. bond] were prepared as factor Xa inhibitors (no data). Thus, 5-cyanoindole was acylated by (COCl)2 and the product converted in 3 steps to 5-cyanoindole-3-acetic acid which was amidated by 4-(2-aminosulfonylphenyl)-2-pyridinamine to give, in 2 addnl. steps, I [R1 = H, R2 = CH2CONHZ1C6H4(SO2NH2)-2, R3 = C(:NH)NH2, Z1 = pyridine-2,4-diyl, dashed line = bond].
IT 202123-90-8P 202123-94-2P 202123-96-4P
202123-97-5P 202123-98-6P 202124-01-4P
202124-04-7P 202124-24-1P 202124-28-5P
202126-86-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amidinoindoles and analogs as factor Xa inhibitors)

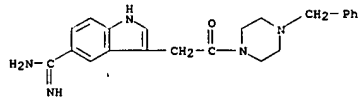
L3 ANSWER 34 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 202123-90-8 CAPLUS
CN Piperazine, 1-[[5-(aminoiminomethyl)-1H-indol-3-yl]acetyl]-4-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)



RN 202123-94-2 CAPLUS
CN Piperazine, 1-[[5-(aminoiminomethyl)-1H-indol-3-yl]acetyl]-4-[(phenylmethyl)sulfonyl]- (9CI) (CA INDEX NAME)

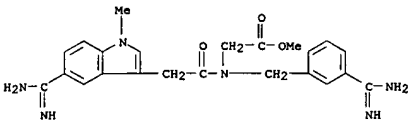


RN 202123-96-4 CAPLUS
CN Piperazine, 1-[[5-(aminoiminomethyl)-1H-indol-3-yl]acetyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)

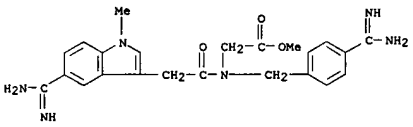


RN 202123-97-5 CAPLUS
CN Glycine, N-[[5-(aminoiminomethyl)-1-methyl-1H-indol-3-yl]acetyl]-N-[[3-(aminoiminomethyl)phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

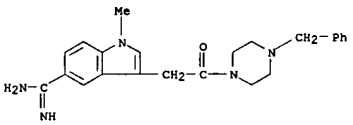
L3 ANSWER 34 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 202123-98-6 CAPLUS
CN Glycine, N-[[5-(aminoiminomethyl)-1-methyl-1H-indol-3-yl]acetyl]-N-[[4-(aminoiminomethyl)phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)



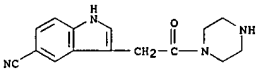
RN 202124-01-4 CAPLUS
CN Piperazine, 1-[[5-(aminoiminomethyl)-1-methyl-1H-indol-3-yl]acetyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 202124-04-7 CAPLUS
CN Piperazine, 1-[[5-(aminoiminomethyl)-1H-indol-3-yl]acetyl]-4-phenyl- (9CI)
(CA INDEX NAME)

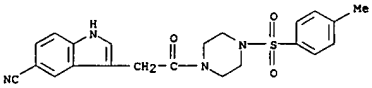
L3 ANSWER 34 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

IT 202124-97-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amidinoindoles and analogs as factor Xa inhibitors)
RN 202124-97-8 CAPLUS
CN Piperazine, 1-[(5-cyano-1H-indol-3-yl)acetyl]-, monohydrochloride (9CI) (CA INDEX NAME)



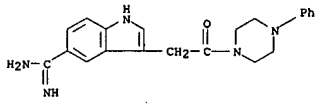
● HCl

IT 202124-91-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amidinoindoles and analogs as factor Xa inhibitors)
RN 202124-91-2 CAPLUS
CN Piperazine,
1-[(5-cyano-1H-indol-3-yl)acetyl]-4-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

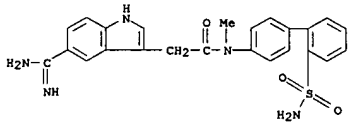


REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

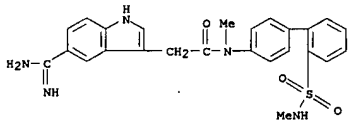
L3 ANSWER 34 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



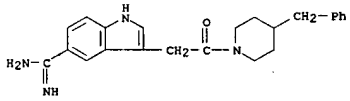
RN 202124-24-1 CAPLUS
CN 1H-Indole-3-acetamide, 5-(aminoiminomethyl)-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-N-methyl- (9CI) (CA INDEX NAME)



RN 202124-28-5 CAPLUS
CN 1H-Indole-3-acetamide, 5-(aminoiminomethyl)-N-methyl-N-[2'-[(methylamino)sulfonyl][1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)



RN 202126-86-1 CAPLUS
CN Piperidine, 1-[[5-(aminoiminomethyl)-1H-indol-3-yl]acetyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 35 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:96240 CAPLUS
DOCUMENT NUMBER: 130:153571
TITLE: Preparation of indole and 2,3-dihydroindole derivatives as potent serotonin reuptake inhibitors and 5-HT1A receptor antagonists
INVENTOR(S): Moltzen, Ejner Knud; Perregaard, Jens Kristian; Mikkelsen, Ivan; Smith, Garrick Paul
PATENT ASSIGNEE(S): H. Lundbeck A/S, Den.
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9905140	A1	19990204	WO 1998-DK336	19980720
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
ZA 9806237	A	19990331	ZA 1998-6237	19980714
CA 2297825	A1	19990204	CA 1998-2297825	19980720
CA 2297825	C	20060314		
AU 9885340	A	19990216	AU 1998-85340	19980720
AU 736596	B2	20010802		
EP 1007523	A1	20000614	EP 1998-936270	19980720
EP 1007523	B1	20031022		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200000231	T2	20000721	TR 2000-200000231	19980720
BR 9810790	A	20000725	BR 1998-10790	19980720
HU 200002830	A2	20010928	HU 2000-2830	19980720
HU 225101	B1	20060629		
NZ 502252	A	20010928	NZ 1998-502252	19980720
JP 2003524571	T	20030819	JP 2000-504136	19980720
IL 133990	A	20030917	IL 1998-133990	19980720
CN 1127501	B	20031112	CN 1998-807554	19980720
AT 252575	T	20031115	AT 1998-936270	19980720
PT 1007523	T	20040227	PT 1998-936270	19980720
ES 2206963	T3	20040516	ES 1998-936270	19980720
CN 1515568	A	20040728	CN 2003-2003106002	19980720
CN 1515569	A	20040728	CN 2003-2003106003	19980720
CZ 295937	B6	20051214	CZ 2000-285	19980720
SK 284866	B6	20060105	SK 2000-95	19980720
PL 190924	B1	20060228	PL 1998-338194	19980720
IN 1998MA01631	A	20050304	IN 1998-MA1631	19980722
NO 2000000372	A	20000321	NO 2000-372	20000125
NO 318610	B1	20050418		
US 6476035	B1	20021105	US 2000-491204	20000125
BG 104148	A	20010531	BG 2000-104148	20000210
BG 64904	B1	20060831		
HK 1030220	A1	20041126	HK 2001-101274	20010221
US 2003018050	A1	20030123	US 2002-223046	20020816

L3 ANSWER 35 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

US 6727263 B2 20040427
PRIORITY APPLN. INFO.: DK 1997-892 A 19970725
US 1997-53713P P 19970725
WO 1998-DK336 W 19980720
US 2000-491204 A3 20000125

OTHER SOURCE(S): MARPAT 130:153571
GI

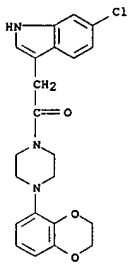
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; X = O, S, CR4R5; Y = CR6R7, CR6R7CR8R9, CR6:CR7; XY = CR4:CR5, CR4:CR5CR6R7; Z = O, S; W = N, C, CH; A = II-IV; R1-R3, R11-R17 = H, halo, CF3, etc.; R4-R9 = H, alkyl; R11 = H, alkyl, alkenyl, etc.] and their salts which are potent serotonin reuptake inhibitors and have 5-HT1A receptor antagonistic activity, were prepared Thus, treatment of 5-chloroindole with oxalyl chloride in Et2O followed by reaction of the resulting 2-(5-chloro-1H-indol-3-yl)-2-oxoacetyl chloride with 1-(1,4-benzodioxan-5-yl)piperazine, and then reduction of the intermediate with LiAlH4 in THF afforded V.oxalate which showed IC50 of 5.0 nM against serotonin reuptake.

IT 220251-80-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indole and 2,3-dihydroindole derivs. as potent serotonin reuptake inhibitors and 5-HT1A receptor antagonists)

RN 220251-80-9 CAPLUS
CN Piperazine, 1-[(6-chloro-1H-indol-3-yl)acetyl]-4-(2,3-dihydro-1,4-benzodioxin-5-yl)- (9CI) (CA INDEX NAME)

L3 ANSWER 35 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 36 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:672540 CAPLUS
DOCUMENT NUMBER: 129:302557
TITLE: Novel 2-[(iminomethyl)amino]phenyl derivatives useful as inhibitors of NO synthase and lipid peroxidation, their preparation, their application as medicines, and pharmaceutical compositions containing them
INVENTOR(S): Chabrier De Lassauniere, Pierre-Etienne; Auvin, Serge; Bigg, Dennis; Auguet, Michel
PATENT ASSIGNEE(S): Societe De Conseils De Recherches Et D'Applications Scientifiques (S.C.R.A.S, Fr.
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9842696	A1	19981001	WO 1998-FR288	19980216
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
FR 2761066	A1	19980925	FR 1997-3528	19970324
FR 2761066	B1	20001124		
CA 2285037	A1	19981001	CA 1998-2285037	19980216
AU 9864043	A	19981020	AU 1998-64043	19980216
AU 733173	B2	20010510		
EP 973763	A1	20000126	EP 1998-909540	19980216
EP 973763	B1	20030528		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO				
BR 9808427	A	20000523	BR 1998-8427	19980216
TR 9902382	T2	20000621	TR 1999-2382	19980216
HU 200001438	A2	20010528	HU 2000-1438	19980216
JP 2001518114	T	20011009	JP 1998-545109	19980216
RU 2183211	C2	20020610	RU 1999-122343	19980216
SK 282773	B6	20021203	SK 1999-1298	19980216
AT 241612	T	20030615	AT 1998-909540	19980216
PT 973763	T	20031031	PT 1998-909540	19980216
ES 2200318	T3	20040301	ES 1998-909540	19980216
IL 131915	A	20040601	IL 1998-131915	19980216
TW 587080	B	20040511	TW 1998-87103327	19980307
ZA 9802203	A	19980916	ZA 1998-2203	19980316
US 6340700	B1	20020122	US 1999-381749	19990922
NO 9904620	A	19991110	NO 1999-4620	19990923
MX 9908724	A	20000630	MX 1999-8724	19990923
US 6335445	B1	20020101	US 1999-456205	19991207
HK 1027563	A1	20050107	HK 2000-106581	20001018
US 2002007062	A1	20020117	US 2001-882264	20010615
US 6630461	B2	20031007		
US 2002045753	A1	20020418	US 2001-945782	20010904

L3 ANSWER 36 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

US 6599903	B2	20030729		
US 2002042511	A1	20020411	US 2001-953682	20010917
US 6586454	B2	20030701		
US 2003078420	A1	20030424	US 2002-191950	20020709
US 6809088	B2	20041026		
US 2005043397	A1	20050224	US 2004-898916	20040726
US 7122535	B2	20061017		
US 2005187272	A1	20050825	US 2005-105291	20050413

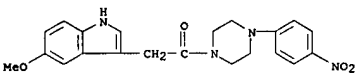
PRIORITY APPLN. INFO.:
FR 1997-3528 A 19970324
FR 1997-7701 A 19970620
WO 1998-FR288 W 19980216
WO 1998-FR1250 W 19980615
US 1999-381749 A2 19990922
US 1999-456205 A3 19991207
US 2001-882264 A3 20010615
US 2002-191950 A3 20020709
US 2004-898916 A3 20040726

OTHER SOURCE(S): MARPAT 129:302557
GI

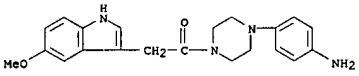
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention concerns novel 2-[(iminomethyl)amino]phenyl derivs., their preparation, their application as medicines, and pharmaceutical compns. containing them. In particular, compds. I [A = radical G1, G2, or G3; R1, R2 = H, OH, alkyl, alkoxy; R3 = H, alkyl, COR4; R4 = alkyl; R5 = H, OH, alkyl, alkoxy; B = alkyl, (un)substituted 5- or 6-membered aryl or heteroaryl (O, S, or N); X = Z1, Z1CO, CH:CHCO, Z1NR3CO, Z1NR3CS, Z1NR3SO2, bond; Y = Z2Q, piperazine, homopiperazine, 2-methylpiperazine, 2,5-dimethylpiperazine, 4-aminopiperidine, NR3Z2Q, NR3COZ2Q, NR3NHCOZ2, NHNHZ2, NR3OZ2, NR3SO2NR3Z2, OZ2Q, OCOZ2Q, or SZ2Q; Q = bond, OZ3, R3NZ3, or SZ3; Z1, Z2, Z3 = bond, alkylene, and preferably (CH2)m; m = 0-6; R6 = H, OH] and salts are claimed. The compds. are inhibitors of NO synthases, and are also antioxidants which inhibit lipid peroxidn. Approx. 60 examples of salts and free bases were prepared and/or claimed. For instance, the benzopyran derivative Trolox® was activated with 1,1'-carbonyldiimidazole and amidated with 1-(4-nitrophenyl)piperazine (79%), followed by hydrogenation of the nitro group to amino (66%), condensation with S-methyl-2-thiophenethiocarboximide hydriodide, and conversion to the HCl salt (40% for 2 steps), to give title compound II.HCl. The IC50 of the latter for inhibiting rat neuronal NO synthase in vitro was < 3.5 μM, and the IC50 for inhibiting rat cerebral lipid peroxidn. in vitro was < 30 μM.

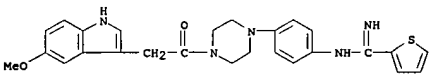
L3 ANSWER 36 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
IT 214124-59-1P 214124-60-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of [(iminomethyl)amino]phenyl derivs. useful as
inhibitors of NO synthase and lipid peroxidn.)
RN 214124-59-1 CAPLUS
CN Piperazine, 1-[(5-methoxy-1H-indol-3-yl)acetyl]-4-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 214124-60-4 CAPLUS
CN Piperazine, 1-(4-aminophenyl)-4-[(5-methoxy-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)



IT 214123-85-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [(iminomethyl)amino]phenyl derivs. useful as inhibitors of
NO synthase and lipid peroxidn.)
RN 214123-85-0 CAPLUS
CN Piperazine, 1-[4-[(imino-2-thienylmethyl)amino]phenyl]-4-[(5-methoxy-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)



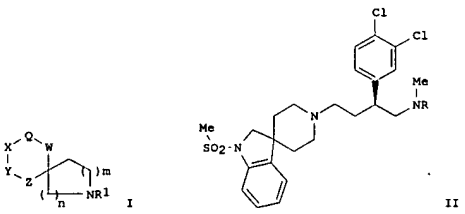
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L3 ANSWER 37 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:402304 CAPLUS
DOCUMENT NUMBER: 129:81760
TITLE: Preparation of spiro-substituted azacycles as modulators of chemokine receptor activity
INVENTOR(S): Mills, Sander G.; Springer, Martin S.; MacCoss, Malcolm
PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Mills, Sander G.; Springer, Martin S.; MacCoss, Malcolm
SOURCE: PCT Int. Appl., 297 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9825605	A1	19980618	WO 1997-US23586	19971212
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9858033	A	19980703	AU 1998-58033	19971212
PRIORITY APPLN. INFO.:			US 1996-32735P P	19961213
			US 1996-33558P P	19961220
			GB 1997-3005 A	19970213
			WO 1997-US23586 W	19971212

OTHER SOURCE(S): MARPAT 129:81760
GI

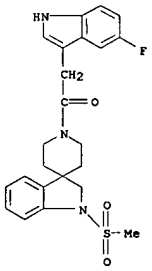
L3 ANSWER 37 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I II

AB Spiroazacycles I [R1 = H, alkyl, aminoalkyl, arylalkyl, etc.; Q = O, S, S(O), SO2, N; W = X bond, alkyl, substituted alkyl, etc.; YZ = fused aryl,
fused heteroaryl; m = n = 0 - 5 and m + n = 1 - 5] were prepared for use as
modulators of chemokine receptor activity (no data). Thus, spiroindoline II (R = 3,5-dimethylbenzoyl) was prepared starting from 3,5-dimethylbenzoic
acid, 1,2-dihydro-1-(methylsulfonyl)spiro[3H-indole-3,4'-piperidine] monohydrochloride, and (S)-3,4-dichloro-N-methyl-β-2-propenylbenzeneethanamine.
IT 167485-09-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of spiro-substituted azacycles as modulators of chemokine receptor activity)
RN 167485-09-8 CAPLUS
CN Spiro[3H-indole-3,4'-piperidine], 1'-[(5-fluoro-1H-indol-3-yl)acetyl]-1,2-dihydro-1-(methylsulfonyl)- (9CI) (CA INDEX NAME)

L3 ANSWER 37 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



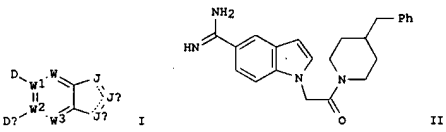
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L3 ANSWER 38 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1998:65894 CAPLUS
DOCUMENT NUMBER: 128:128015
TITLE: Preparation of amidinoindoles and amidinoazoles as inhibitors of factor Xa and of thrombin
INVENTOR(S): Dominguez, Celia; Han, Qi; Duffy, Daniel Emmett; Park, Jeongsook Maria; Quan, Mimi Lifen; Rossi, Karen Anita; Wexler, Ruth Richmond
PATENT ASSIGNEE(S): Du Pont Merck Pharmaceutical Co., USA
SOURCE: PCT Int. Appl., 176 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9801428	A1	19980115	WO 1997-US11325	19970630
W: AM, AU, AZ, BR, BY, CA, CN, CZ, EE, HU, IL, JP, KG, KR, KZ, LT, LV, MD, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, UA, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2259573	A1	19980115	CA 1997-2259573	19970630
AU 9736456	A	19980202	AU 1997-36456	19970630
EP 960102	A1	19991201	EP 1997-933214	19970630
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
NZ 333696	A	20000623	NZ 1997-333696	19970630

PRIORITY APPLN. INFO.: US 1996-676766 A 19960708
US 1997-49519P P 19970613
WO 1997-US11325 W 19970630

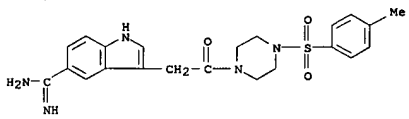
OTHER SOURCE(S): MARPAT 128:128015
GI



I II

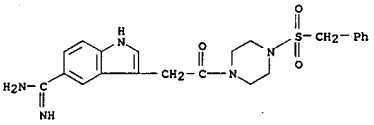
AB The title compds. {I; W, W3 = CH, N; W1, W2 = C, CH, N (provided that one of W1 and W2 is C(C(=NH)NH2) and at most two of W, W1, W2, and W3 are N); one of D, Da = H, C1-4 alkoxy, CN, etc. and the other is absent; one of Ja

L3 ANSWER 38 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
and Jb is substituted by -(CH2)n-Z-A-B; J, Ja, Jb combine to form an arom. heterocyclic system contg. from 1-2 heteroatoms (N, O, and S), a heterocyclic ring wherein Jb = N and J and Ja = (un)substituted CH2, a heterocyclic ring wherein Jb = CH, J = (un)substituted NH and Ja = (un)substituted CH; Z = CH:CH, SO2CH2, etc.; A = (un)substituted PhCH2, PhCH2CH2, etc.; B = C3-6 alkyl, (un)substituted PhCH2, 5-10 membered heterocyclic system, etc.}, useful as inhibitors of factor Xa or thrombin, were prepd. and formulated. Thus, reaction of 5-cyanoindole-1-acetic acid with 4-benzylpiperidine followed by treatment of the resulting 1-(4-benzylpiperidinocarbonyl)methyl-5-cyanoindole with HCl(g) in MeOH, and then with (NH4)2CO3 in MeOH afforded the title compd. II. Some compds. I were evaluated and showed Ki of < 5 μM against thrombin.
IT 202123-90-8P 202123-94-2P 202123-96-4P
202123-97-5P 202123-98-6P 202124-01-4P
202124-04-7P 202124-24-1P 202124-28-5P
202126-86-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amidinoindoles and amidinoazoles as inhibitors of factor Xa and of thrombin)
RN 202123-90-8 CAPLUS
CN Piperazine, 1-[[5-(aminoiminomethyl)-1H-indol-3-yl]acetyl]-4-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

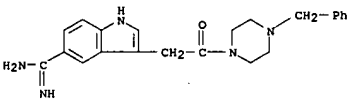


RN 202123-94-2 CAPLUS
CN Piperazine, 1-[[5-(aminoiminomethyl)-1H-indol-3-yl]acetyl]-4-[(phenylmethyl)sulfonyl]- (9CI) (CA INDEX NAME)

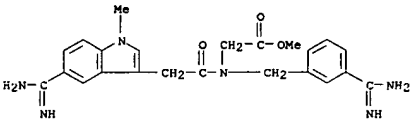
L3 ANSWER 38 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



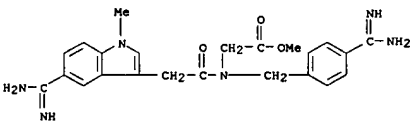
RN 202123-96-4 CAPLUS
CN Piperazine, 1-[[5-(aminoiminomethyl)-1H-indol-3-yl]acetyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 202123-97-5 CAPLUS
CN Glycine, N-[[5-(aminoiminomethyl)-1-methyl-1H-indol-3-yl]acetyl]-N-[[3-(aminoiminomethyl)phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

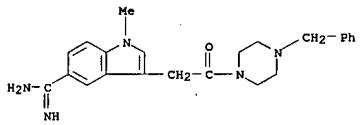


RN 202123-98-6 CAPLUS
CN Glycine, N-[[5-(aminoiminomethyl)-1-methyl-1H-indol-3-yl]acetyl]-N-[[4-(aminoiminomethyl)phenyl]methyl]-, methyl ester (9CI) (CA INDEX NAME)

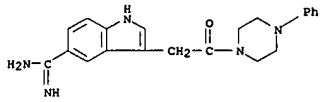


RN 202124-01-4 CAPLUS

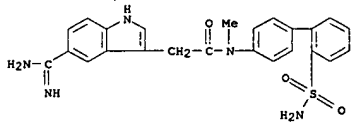
L3 ANSWER 38 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN Piperazine, 1-[[5-(aminoiminomethyl)-1-methyl-1H-indol-3-yl]acetyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 202124-04-7 CAPLUS
CN Piperazine, 1-[[5-(aminoiminomethyl)-1H-indol-3-yl]acetyl]-4-phenyl- (9CI)
(CA INDEX NAME)

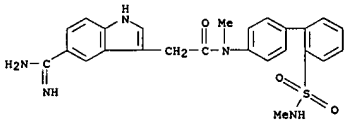


RN 202124-24-1 CAPLUS
CN 1H-Indole-3-acetamide, 5-(aminoiminomethyl)-N-[2'-(aminosulfonyl)[1,1'-biphenyl]-4-yl]-N-methyl- (9CI) (CA INDEX NAME)

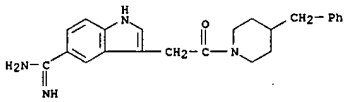


RN 202124-28-5 CAPLUS
CN 1H-Indole-3-acetamide, 5-(aminoiminomethyl)-N-methyl-N-[2'-[(methylamino)sulfonyl][1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

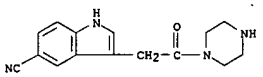
L3 ANSWER 38 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 202126-86-1 CAPLUS
CN Piperidine, 1-[[5-(aminoiminomethyl)-1H-indol-3-yl]acetyl]-4-(phenylmethyl)- (9CI) (CA INDEX NAME)



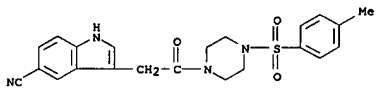
IT 202124-97-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of amidinoindoles and amidinoazoles as inhibitors of factor Xa
and of thrombin)
RN 202124-97-8 CAPLUS
CN Piperazine, 1-[(5-cyano-1H-indol-3-yl)acetyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

IT 202124-91-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of amidinoindoles and amidinoazoles as inhibitors of factor Xa
and of thrombin)
RN 202124-91-2 CAPLUS
CN Piperazine, 1-[(5-cyano-1H-indol-3-yl)acetyl]-4-[(4-methylphenyl)sulfonyl]-

L3 ANSWER 38 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

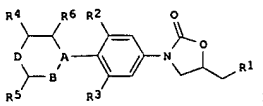
L3 ANSWER 39 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:579718 CAPLUS
DOCUMENT NUMBER: 127:248104
TITLE: Preparation of aryloxooxazolidinylmethylacetamides and related compounds as antibacterials.
INVENTOR(S): Gravestock, Michael Barry
PATENT ASSIGNEE(S): Zeneca Ltd., UK; Gravestock, Michael Barry
SOURCE: PCT Int. Appl., 111 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9730995	A1	19970828	WO 1997-GB462	19970220
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
ZA 9701469	A	19970825	ZA 1997-1469	19970220
AU 9718053	A	19970910	AU 1997-18053	19970220
EP 882042	A1	19981209	EP 1997-903509	19970220
R: CH, DE, FR, GB, IT, LI				
JP 11514662	T	19991214	JP 1997-529888	19970220
US 5981528	A	19991109	US 1997-945160	19971021
US 6271383	B1	20010807	US 1999-364389	19990730
US 6365751	B1	20020402	US 2001-836095	20010417

PRIORITY APPLN. INFO.: GB 1996-3939 A 19960224
GB 1996-18404 A 19960904
WO 1997-GB462 W 19970220
US 1997-945160 A3 19971021
US 1999-364389 A3 19990730

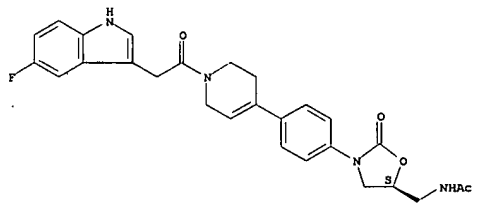
OTHER SOURCE(S): MARPAT 127:248104
GI



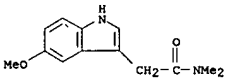
I

L3 ANSWER 39 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
AB Title compds. (I; R1 = OH, Cl, Br, F, alkylsulfonyloxy, amino, N3, alkoxy,
alkylthio, alkylaminocarbonyloxy, etc.; R2, R3 = H, F; D = O, S, SO, SO2, imino, acylimino; R4, R5 = H, Br, O, alkyl, alkanoylaminoalkyl, hydroxyalkyl, CO2H, alkoxycarbonyl, etc.; R6 = H, alkyl, OH, alkoxy, alkanoyloxy; AB = C:CRa, CHCHRa, or C(OH)CHRa; Ra = H, alkyl), were prepared
Thus, a mixture of tert-Bu 1,2,3,6-tetrahydro-4-(trifluoromethylsulfonyloxy)pyridine-1-carboxylate, Pd2(dibenzylideneacetone)2, Ph3As, and LiCl in N-methylpyrrolidine was treated with (S)-5-acetamidomethyl-3-(4-trimethyltinphenyl)oxazolidin-2-one (preparation given) followed by stirring at room temperature to 40° to
give 23% (S)-N-[3-[4-(1-tert-butyloxycarbonyl-1,2,5,6-tetrahydropyrid-4-yl)phenyl]-2-oxooxazolidin-5-ylmethyl]acetamide. The latter showed a min.
inhibitory concentration of 1.0 μg/mL against Staphylococcus aureus Oxford.
IT 195816-92-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of aryloxooxazolidinylmethylacetamides and related compds. as
antibacterials)
RN 195816-92-3 CAPLUS
CN Acetamide, N-[[3-[4-[1-[(5-fluoro-1H-indol-3-yl)acetyl]-1,2,3,6-tetrahydro-4-pyridinyl]phenyl]-2-oxo-5-oxazolidinyl]methyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 40 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:507924 CAPLUS
DOCUMENT NUMBER: 127:190580
TITLE: Synthesis of iodine 131 derivatives of indolealkylamines for brain mapping
AUTHOR(S): Sintas, Jose A.; Vitale, Arturo A.
CORPORATE SOURCE: Departamento de Quimica Organica, Faculted de Ciencias
Exactas y Naturales, PROPLAME-CONICET, Universidad de Buenos Aires, Buenos Aires, 1428, Argent.
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1997), 39(8), 677-684
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The synthesis and spectral properties of new radioiodinated indolealkylamines like 2-[131I]-iodo-N,N-dimethyltryptamine, 2-[131I]-iodo-N-methyltryptamine, 2-[131I]-iodo-5-methoxy-N,N-dimethyltryptamine, 2-[131I]-iodo-5-hydroxy-N,N-dimethyltryptamine (2-[131I]-iodobufotenine), and 2-[131I]-iodotryptamine and the known 2-[131I]-iodo-N-acetyl-5-methoxytryptamine (2-[131I]-iodomelatonin) are described. The radioiodinated compds. were synthesized via a high-yield novel method, and their spectral properties are fully described. These compds. are of biol. importance and can be used for brain mapping with SPECT technol.
IT 151290-19-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 131I derivs. of indolealkylamines for brain mapping)
RN 151290-19-6 CAPLUS
CN 1H-Indole-3-acetamide, 5-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)



L3 ANSWER 41 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1997:456960 CAPLUS
DOCUMENT NUMBER: 127:95194
TITLE: New benzisoindole derivatives as inhibitors of farnesyl transferase, their preparation, and pharmaceutical compositions containing them.
INVENTOR(S): Commercon, Alain; Lebrun, Alain; Mailliet, Patrick; Peyronel, Jean Francois; Sounigo, Fabienne; Truchon, Alain; Zucco, Martine; Cheve, Michel
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer SA, Fr.
SOURCE: Fr. Demande, 96 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2736641	A1	19970117	FR 1995-8296	19950710
FR 2736641	B1	19970822		
TW 438792	B	20010607	TW 1996-85108158	19960705
CA 2224414	A1	19970130	CA 1996-2224414	19960708
WO 9703050	A1	19970130	WO 1996-FR1062	19960708
W: AL, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KP, KR, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9665224	A	19970210	AU 1996-65224	19960708
AU 712194	B2	19991028		
EP 839133	A1	19980506	EP 1996-924952	19960708
EP 839133	B1	19991006		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
CN 1190389	A	19980812	CN 1996-195415	19960708
CN 1096448	B	20021218		
JP 11511123	T	19990928	JP 1996-505557	19960708
AT 185341	T	19991015	AT 1996-924952	19960708
ES 2139373	T3	20000201	ES 1996-924952	19960708
IL 122812	A	20010430	IL 1996-122812	19960708
SK 282250	B6	20011203	SK 1998-26	19960708
CZ 291620	B6	20030416	CZ 1998-54	19960708
ZA 9605868	A	19970129	ZA 1996-5868	19960710
BR 9609440	A	19990629	BR 1996-9440	19960710
NO 9800094	A	19980217	NO 1998-94	19980109
NO 309565	B1	20010219		
US 5936097	A	19990810	US 1998-981840	19980723
GR 3031409	T3	20000131	GR 1999-402001	19991007
PRIORITY APPLN. INFO.:			FR 1995-8296 A	19950710
			WO 1996-FR1062 W	19960708

OTHER SOURCE(S): MARPAT 127:95194
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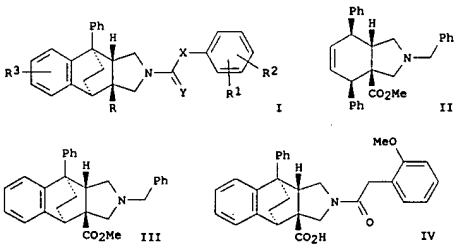
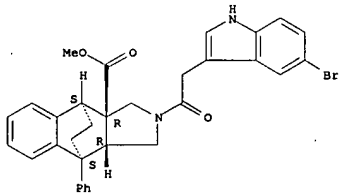
L3 ANSWER 41 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



AB Title compds. I [R = (un)substituted (CH2)mX1(CH2)nZ; X1 = bond, O, S; m = 0-1; n = 0-2; Z = CO2H, alkoxycarbonyl, (un)substituted carbamoyl, etc.; R1, R2 = H, halo, alkyl, (un)substituted alkoxy; or R1R2 form (un)saturated heterocycle; or R2 forms dimer via disulfide bridge; R3 = H, halo, alkyl, alkenyl, alkoxy, alkylthio; X = O, S, NH, CO, CH2, CH2CH2, alkylene, 1,1-cycloalkanediyl; Y = O, S], in racemic form or as optical isomers, are claimed. The compds. are inhibitors of farnesyl transferase, and show marked antitumor and antileukemic properties. For example, cis-3,6-diphenyl-1,4-cyclohexadienecarboxylic acid Me ester (preparation given) reacted with PhCH2N(CH2OBu)(CH2SiMe3) in refluxing CF3CO2H to give the intermediate hexahydroisoindole derivative II.HCl, which was further cyclized by CF3SO3H at 5-20° to give the benz[f]isoindole intermediate III. This was then converted in 3 steps to title compound IV. In an assay for inhibition of farnesyl transferase, IV had an IC50 of 0.31 μM.
IT 191989-96-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of new benzisoindole derivs. farnesyl transferase inhibitors)
RN 191989-96-5 CAPLUS
CN 4,9-Ethano-3aH-benz[f]isoindole-3a-carboxylic acid, 2-[(5-bromo-1H-indol-3-yl)acetyl]-1,2,3,4,9,9a-hexahydro-9-phenyl-, methyl ester, (3aα,4β,9α,9aα)- (9CI) (CA INDEX NAME)

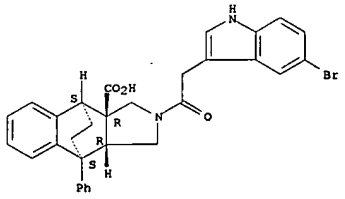
Relative stereochemistry.

L3 ANSWER 41 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



IT 191989-23-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of new benzisoindole derivs. farnesyl transferase inhibitors)
RN 191989-23-8 CAPLUS
CN 4,9-Ethano-3aH-benz[f]isoindole-3a-carboxylic acid, 2-[(5-bromo-1H-indol-3-yl)acetyl]-1,2,3,4,9,9a-hexahydro-9-phenyl-, (3aα,4β,9α,9aα)- (9CI) (CA INDEX NAME)

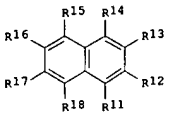
Relative stereochemistry.

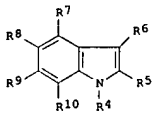


L3 ANSWER 42 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:1006753 CAPLUS
DOCUMENT NUMBER: 124:175829
TITLE: Substituted naphthalene and indole compounds exhibiting selective leukotriene B4 antagonist activity
INVENTOR(S): Huang, Fu Chih; Chan, Wan K.; Sutherland, Charles A.; Galemmo, Jr Robert A.
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer Pharmaceuticals Inc., USA
SOURCE: U.S., 26 pp. Cont.-in-part of U.S. Ser. No. 580,243, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5468898	A	19951121	US 1993-777246	19930423
WO 9204321	A1	19920319	WO 1991-US6447	19910906
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
PRIORITY APPLN. INFO.:			US 1990-580243	B2 19900910
			WO 1991-US6447	W 19910906

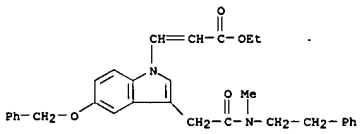
OTHER SOURCE(S): MARPAT 124:175829
GI


I


II

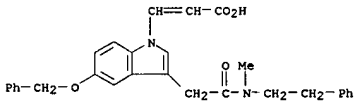
AB This invention relates to naphthalene and indole derivs. I and II, resp., containing an amido substituent, a substituent group having a terminal carboxylic acid or derivative thereof and a lipophilic substituent [i.e., at least one of R4, R5, R6, R7, R8, R9 and R10 and R11, R12, R13, R14, R15, R16, R17, R18 are A(CR2)aCONR'(CR2)bB; at least one of R4, R5, R6, R7, R8, R9 and R10 and R11, R12, R13, R14, R15, R16, R17, R18 are (CR2)dD(CR2)eE; and at least one of R4, R5, R6, R7, R8, R9 and R10 and R11, R12, R13, R14, R15, R16, R17, R18 are (CR2)fF(CR2)gG and the remaining R4, R5, R6, R7, R8, R9 and R10 and R11, R12, R13, R14, R15, R16, R17, R18 are H; where A is CRR or O; B and G are (un)substituted Ph; D = e.g., bond, O, CRR; E = e.g., CO2R', CONR'R'; F = e.g., bond, O, CRR; R = e.g., H; R' = e.g., H,

L3 ANSWER 42 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
alkyl; a, b, d, e, f, and g are independently 0-4] having selective LTB4 antagonist properties (no data) and to methods for the treatment of disorders which result from LTB4 activity and pharmaceutical compns. including such compds. Thus, e.g., amidation of bromoacetyl chloride with N-methyl-N-phenethylamine afforded N-methyl-N-phenethyl-2-bromoacetamide which was used to alkylate 5-hydroxyindole, thus affording 5-[2-(N-methyl-N-phenethyl)amino-2-oxoethoxy]indole; formylation of the latter afforded 5-[2-(N-methyl-N-phenethyl)amino-2-oxoethoxy]indole-3-carboxaldehyde; N-alkylation of the latter with N-methyl-N-phenethyl-2-bromoacetamide afforded N-methyl-N-phenethyl-2-[(5-(2-methylphenethylamino-2-oxoethoxy)-3-formyl)indol-1-yl]acetamide; condensation of the latter with tri-Et phosphonoacetate afforded N-methyl-N-phenethyl-2-[3-(2-carbethoxyvinyl)-5-(2-(N-methyl-N-phenethyl)amino-2-oxoethoxy)indol-1-yl]acetamide.
IT 141835-69-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(substituted naphthalene and indole compds. exhibiting selective leukotriene B4 antagonist activity)
RN 141835-69-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[2-[methyl(2-phenylethyl)amino]-2-oxoethyl]-5-(phenylmethoxy)-1H-indol-1-yl]-, ethyl ester (9CI) (CA INDEX NAME)

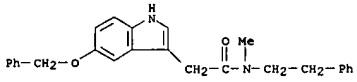


IT 141835-21-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(substituted naphthalene and indole compds. exhibiting selective leukotriene B4 antagonist activity)
RN 141835-21-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[2-[methyl(2-phenylethyl)amino]-2-oxoethyl]-5-(phenylmethoxy)-1H-indol-1-yl]- (9CI) (CA INDEX NAME)

L3 ANSWER 42 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



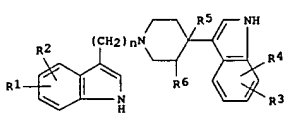
IT 141835-68-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(substituted naphthalene and indole compds. exhibiting selective leukotriene B4 antagonist activity)
RN 141835-68-9 CAPLUS
CN 1H-Indole-3-acetamide, N-methyl-N-(2-phenylethyl)-5-(phenylmethoxy)-(9CI)
(CA INDEX NAME)



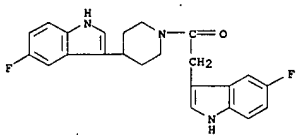
L3 ANSWER 43 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:995279 CAPLUS
DOCUMENT NUMBER: 124:145907
TITLE: Preparation of 1-(3-indolylalkyl)-4-(3-indolyl)piperidines as dopamine agonists or antagonists.
INVENTOR(S): Boettcher, Henning; Maerz, Joachim; Seyfried, Christoph; Greiner, Hartmut; Bartoszyk, Gerd
PATENT ASSIGNEE(S): Merck Patent GmbH, Germany
SOURCE: Ger. Offen., 14 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 4414113	A1	19951026	DE 1994-4414113	19940422
EP 683166	A1	19951122	EP 1995-105227	19950407
EP 683166	B1	19981028		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 172730	T	19981115	AT 1995-105227	19950407
ES 2125508	T3	19990301	ES 1995-105227	19950407
AU 9516488	A	19951102	AU 1995-16488	19950413
AU 697749	B2	19981015		
JP 07291969	A	19951107	JP 1995-91077	19950417
SK 280881	B6	20000814	SK 1995-508	19950419
CA 2147451	A1	19951023	CA 1995-2147451	19950420
CA 2147451	C	20060328		
CN 1114651	A	19960110	CN 1995-104705	19950420
CN 1047385	B	19991215		
TW 401416	B	20000811	TW 1995-84103916	19950420
NO 9501529	A	19951023	NO 1995-1529	19950421
NO 307831	B1	20000605		
ZA 9503260	A	19960109	ZA 1995-3260	19950421
HU 74096	A2	19961128	HU 1995-1139	19950421
US 5693655	A	19971202	US 1995-426405	19950421
CZ 285369	B6	19990714	CZ 1995-1035	19950421
RU 2151148	C1	20000620	RU 1995-106675	19950421
PL 180781	B1	20010430	PL 1995-308287	19950421
PRIORITY APPLN. INFO.:			DE 1994-4414113 A	19940422

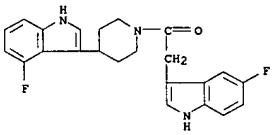
OTHER SOURCE(S): MARPAT 124:145907
GI


I

L3 ANSWER 43 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
AB Title compds. [I; R1-R4 = H, alkyl, OH, alkoxy, F, Cl, Br, iodo, cyano, CF3, CO2H, CONH2, alkoxycarbonyl, etc.; R1R2, R3R4 = OCH2O; R5 = H, OH; R6 = H; R5R6 = bond; n = 2-6], were prepared as drugs (no data). Thus, 3-(4-chlorobutyl)-5-methoxyindole and 4-(3-indolyl)piperidine were refluxed 8 h in MeCN to give 3-[1-[4-(5-methoxyindol-3-yl)butyl]-4-piperidinyl]indole hydrochloride.
IT 173150-68-0 173150-69-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 1-(3-indolylalkyl)-4-(3-indolyl)piperidines as dopamine agonists or antagonists)
RN 173150-68-0 CAPLUS
CN Piperidine, 4-(5-fluoro-1H-indol-3-yl)-1-[(5-fluoro-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)

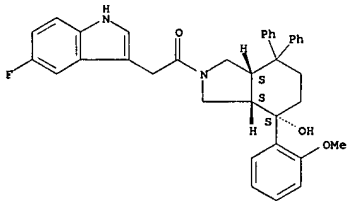


RN 173150-69-1 CAPLUS
CN Piperidine, 4-(4-fluoro-1H-indol-3-yl)-1-[(5-fluoro-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)



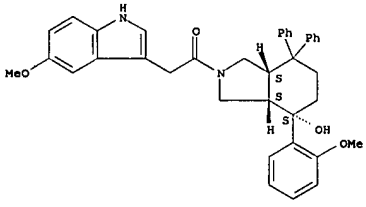
L3 ANSWER 44 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Isoindol-4-ol, 2-[(5-fluoro-1H-indol-3-yl)acetyl]octahydro-4-(2-methoxyphenyl)-7,7-diphenyl-, [3aS-(3aα,4β,7aα)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 153438-64-3 CAPLUS
CN 1H-Isoindol-4-ol, octahydro-2-[(5-methoxy-1H-indol-3-yl)acetyl]-4-(2-methoxyphenyl)-7,7-diphenyl-, [3aS-(3aα,4β,7aα)]- (9CI) (CA INDEX NAME)

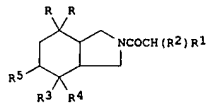
Absolute stereochemistry.



L3 ANSWER 44 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:851691 CAPLUS
DOCUMENT NUMBER: 123:285765
TITLE: Preparation of perhydroisoindole antiemetics
INVENTOR(S): Garret, Claude; Louvel, Erik
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer S.A., Fr.
SOURCE: PCT Int. Appl., 62 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9509628	A1	19950413	WO 1994-FR1160	19941005
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, NO, NZ, PL, RO, RU, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
FR 2710842	A1	19950414	FR 1993-11945	19931007
FR 2710842	B1	19951124		
AU 9478581	A	19950501	AU 1994-78581	19941005
PRIORITY APPLN. INFO.:			FR 1993-11945 A	19931007
			WO 1994-FR1160 W	19941005

OTHER SOURCE(S): MARPAT 123:285765
GI



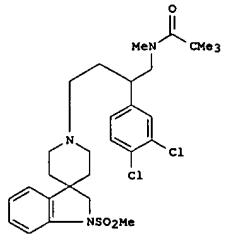
I

AB The title compds. [I; R = (un)substituted Ph; R1 = (un)substituted Ph, cyclohexadienyl, naphthyl, indenyl, (un)substituted heterocyclyl; R2 = H, halogen, OH, alkyl, aminoalkyl, alkylaminoalkyl, dialkylaminoalkyl, alkyloxy, alkylthio, acyloxy, CO2H, (un)substituted alkyloxycarbonyl, benzyloxycarbonyl, NH2, acylamino; R3 = (un)substituted Ph; R4 = OH or F if R5 = H; etc.] [e.g., (3aS,4S,7aS)-7,7-diphenyl-4-(2-methoxyphenyl)-2-tert-butoxycarbonyl-4-perhydroisoindolol], useful as antiemetics, are prepared and I-containing formulations presented.
IT 153438-63-2P 153438-64-3P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of perhydroisoindole antiemetics)
RN 153438-63-2 CAPLUS

L3 ANSWER 45 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1995:781772 CAPLUS
DOCUMENT NUMBER: 123:169671
TITLE: Preparation of spirocyclic compounds as neurokinin antagonists
INVENTOR(S): MacCoss, Malcolm; Mills, Sander G.; Shah, Shrenik K.; Chiang, Yuan-Ching P.; Dunn, Patrick T.; Koyama, Hiroo; Finke, Paul E.; Qi, Hongbo; Robichaud, Albert J.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: PCT Int. Appl., 226 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9429309	A1	19941222	WO 1994-US5545	19940517
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SI, SK, TT, UA, US, UZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2163995	A1	19941222	CA 1994-2163995	19940517
AU 9472011	A	19950103	AU 1994-72011	19940517
AU 680020	B2	19970717		
EP 702681	A1	19960327	EP 1995-901979	19940517
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 08511522	T	19961203	JP 1994-501802	19940517
ZA 9403946	A	19950120	ZA 1994-3946	19940606
PRIORITY APPLN. INFO.:			US 1993-72904 A	19930607
			WO 1994-US5545 W	19940517

OTHER SOURCE(S): MARPAT 123:169671
GI



I

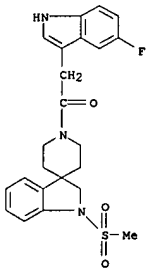
L3 ANSWER 45 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB Spirocyclic nitrogen-heterocyclic compds. were disclosed as tachykinin receptor antagonists useful for the treatment of inflammatory diseases, pain or migraine, and asthma. In particular, said compds. were shown to be neurokinin antagonists. Many example compds. are claimed. One such specific compound is N-[3-(3,4-dichlorophenyl)-4-[1,2-dihydro-1-(sulfonylmethyl)spiro[3H-indole-3,4'-piperidin]-1'-yl]butyl]-2,2-dimethylpropanamide (I).

IT 167485-09-8P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of spirocyclic compds. as kinin receptor antagonists)

RN 167485-09-8 CAPLUS

CN Spiro[3H-indole-3,4'-piperidine], 1'-[(5-fluoro-1H-indol-3-yl)acetyl]-1,2-dihydro-1-(methylsulfonyl)- (9CI) (CA INDEX NAME)



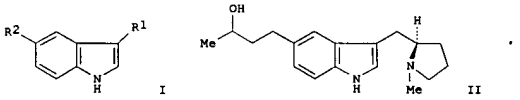
L3 ANSWER 46 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:772570 CAPLUS
DOCUMENT NUMBER: 123:169499
TITLE: Indole derivatives as 5-HT1-like agonists for use in migraine
INVENTOR(S): Wythes, Martin James
PATENT ASSIGNEE(S): Pfizer Ltd., UK; Pfizer Inc.; Pfizer Research and Development Company, N.V./S.A.
SOURCE: PCT Int. Appl., 124 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9424127	A1	19941027	WO 1994-EP1121	19940411
W: AU, BR, CA, CN, CZ, FI, HU, JP, KR, NO, NZ, PL, RU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2157397	A1	19941027	CA 1994-2157397	19940411
CA 2157397	C	19990706		
AU 9465670	A	19941108	AU 1994-65670	19940411
BR 9406481	A	19960109	BR 1994-6481	19940411
EP 695301	A1	19960207	EP 1994-913573	19940411
EP 695301	B1	19961030		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
CN 1121348	A	19960424	CN 1994-191850	19940411
JP 08507083	T	19960730	JP 1994-522726	19940411
HU 73807	A2	19960930	HU 1995-1920	19940411
AT 144773	T	19961115	AT 1994-913573	19940411
ES 2094653	T3	19970116	ES 1994-913573	19940411
ZA 9402722	A	19951020	ZA 1994-2722	19940420
FI 9504944	A	19951017	FI 1995-4944	19951017
NO 9504168	A	19951019	NO 1995-4168	19951019
US 5607960	A	19970304	US 1995-532573	19951020

PRIORITY APPLN. INFO.: GB 1993-8360 A 19930422
GB 1993-24433 A 19931127
WO 1994-EP1121 W 19940411

OTHER SOURCE(S): MARPAT 123:169499
GI



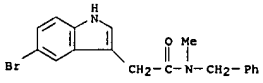
L3 ANSWER 46 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

AB The title compds., 3-(pyrrolidinylmethyl)indoles and 3-(piperidinylmethyl)indoles I [R1 = (2-pyrrolidinyl)methyl, 3-pyrrolidinyl, 4-piperidinyl, (3-piperidinyl)methyl; R2 = alkyl, oxoalkyl, etc.] were disclosed as selective 5-HT1-like agonists useful in the treatment of migraine, cluster headache, chronic paroxysmal hemicrania and headache associated with vascular disorders. A specifically claimed example compound is 5-(3-hydroxybutyl)-3-[(R)-(1-methyl-2-pyrrolidinyl)methyl]-1-H-indole (II).

IT 167303-72-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (aminoalkyl)indoles 5-HT1-like agonists)

RN 167303-72-2 CAPLUS

CN 1H-Indole-3-acetamide, 5-bromo-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



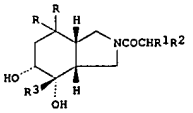
L3 ANSWER 47 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1995:615038 CAPLUS
DOCUMENT NUMBER: 123:32956
TITLE: Preparation of pharmaceutical perhydroisoindole derivatives as neurokinin A antagonists
INVENTOR(S): Crespo, Andre; Fardin, Veronique; Guillaume, Jean-Marc; Malleron, Jean -Luc; Peyronel, Jean-Francois
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer S.A., Fr.
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9422822	A1	19941013	WO 1994-FR371	19940401
W: AU, CA, CZ, FI, HU, JP, KR, NO, NZ, PL, RU, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
FR 2703679	A1	19941014	FR 1993-3965	19930405
FR 2703679	B1	19950623		
CA 2158663	A1	19941013	CA 1994-2158663	19940401
AU 9465068	A	19941024	AU 1994-65068	19940401
EP 693059	A1	19960124	EP 1994-912582	19940401
EP 693059	B1	19970312		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 08508283	T	19960903	JP 1994-521762	19940401
HU 74089	A2	19961128	HU 1995-2902	19940401
AT 150014	T	19970315	AT 1994-912582	19940401
ES 2099601	T3	19970516	ES 1994-912582	19940401
US 5631279	A	19970520	US 1995-448402	19950607
NO 9503913	A	19951002	NO 1995-3913	19951002
FI 9504730	A	19951117	FI 1995-4730	19951004

PRIORITY APPLN. INFO.: FR 1993-3965 A 19930405
WO 1994-FR371 W 19940401

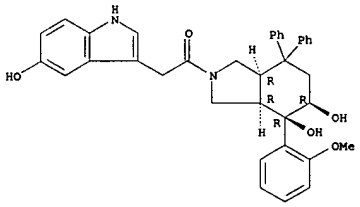
OTHER SOURCE(S): MARPAT 123:32956
GI



AB Title compds. I (R = (substituted)Ph; R1 = (substituted)Ph, PhCh2O, (substituted)-C1-4 alkyl, (substituted)amino, (substituted)heterocyclyl, cyclohexadienyl, naphthyl, indenyl; R2 = H, halo, HO, alkyl, aminoalkyl, allylaminoalkyl, dialkylaminoalkyl, etc.; R3 = (substituted)Ph), are prepared (3AR,4R,5R,7aR)-7,7-diphenyl-4-(2-methoxyphenyl)perhydro-4,5-isoindolediol (preparation given) and 3-indolylacetic acid in CH2Cl2

L3 ANSWER 47 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
to 1-benzotriazolylol hydrate, 1-(3-dimethylaminopropyl)-3-ethylcarbodiimide and diisopropylethylamine to give (3aR,4R,5R,7aR)-I (R1 = 3-indolyl, R2 = H, R3 = 2-(MeO)C6H4) which at 10-1000 nM on human receptor NK2 showed IC50 of 215 nM. A formulation tablet comprising I is given.
IT 163838-54-8P 163838-57-1P 163838-58-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pharmaceutical perhydroisoindole derivs. as neurokinin A antagonists)
RN 163838-54-8 CAPLUS
CN 1H-Isoindole-4,5-diol, octahydro-2-[(5-hydroxy-1H-indol-3-yl)acetyl]-4-(2-methoxyphenyl)-7,7-diphenyl-, (3aR-(3aα,4β,5β,7aα)]-(9CI) (CA INDEX NAME)

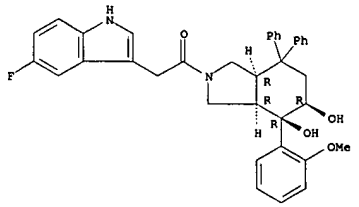
Absolute stereochemistry.



RN 163838-57-1 CAPLUS
CN 1H-Isoindole-4,5-diol, 2-[(5-fluoro-1H-indol-3-yl)acetyl]octahydro-4-(2-methoxyphenyl)-7,7-diphenyl-, (3aα,4β,5β,7aα)- (9CI) (CA INDEX NAME)

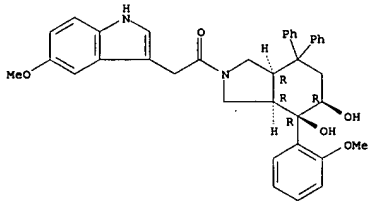
Relative stereochemistry.

L3 ANSWER 47 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



RN 163838-58-2 CAPLUS
CN 1H-Isoindole-4,5-diol, octahydro-2-[(5-methoxy-1H-indol-3-yl)acetyl]-4-(2-methoxyphenyl)-7,7-diphenyl-, (3aα,4β,5β,7aα)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L3 ANSWER 48 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

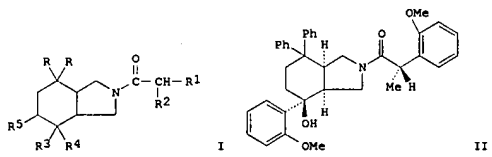
ACCESSION NUMBER:	1994:270102 CAPLUS
DOCUMENT NUMBER:	120:270102
TITLE:	Perhydroisoindole derivatives as substance P antagonists and their preparation
INVENTOR(S):	Achard, Daniel; Grisoni, Serge; Malleron, Jean Luc; Peyronel, Jean-francois; Tabart, Michel
PATENT ASSIGNEE(S):	Rhone-Poulenc Rorer S.A., Fr.
SOURCE:	PCT Int. Appl., 67 pp. CODEN: PIXXD2
DOCUMENT TYPE:	Patent
LANGUAGE:	French
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9321155	A1	19931028	WO 1993-FR352	19930408
W: AU, CA, CZ, FI, HU, JP, KR, KZ, NO, NZ, PL, RU, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
FR 2689888	A1	19931015	FR 1992-4390	19920410
FR 2689888	B1	19940610		
IL 105255	A	19970218	IL 1993-105255	19930401
ZA 9302527	A	19931108	ZA 1993-2527	19930408
AU 9339565	A	19931118	AU 1993-39565	19930408
AU 667214	B2	19960314		
EP 635003	A1	19950125	EP 1993-909005	19930408
EP 635003	B1	19980617		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07505410	T	19950615	JP 1993-518041	19930408
JP 3205557	B2	20010904		
HU 71354	A2	19951128	HU 1994-2911	19930408
PL 172754	B1	19971128	PL 1993-305360	19930408
SK 279032	B6	19980506	SK 1994-1220	19930408
AT 167472	T	19980715	AT 1993-909005	19930408
CZ 284213	B6	19980916	CZ 1994-2482	19930408
ES 2118232	T3	19980916	ES 1993-909005	19930408
RU 2127260	C1	19990310	RU 1994-45855	19930408
NO 9403692	A	19941003	NO 1994-3692	19941003
FI 9404729	A	19941007	FI 1994-4729	19941007
FI 105023	B1	20000531		
US 5484804	A	19960116	US 1994-313121	19941011
PRIORITY APPLN. INFO.:			FR 1992-4390 A	19920410
			WO 1993-FR352 A	19930408

OTHER SOURCE(S): MARPAT 120:270102
GI

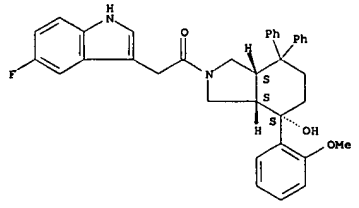
L3 ANSWER 48 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I II

AB Title compds. I [R = Ph optionally substituted with halogen or Me in position 2 or 3; R1 = (un)substituted Ph, cyclohexadienyl, naphthyl, indenyl, heterocyclyl; R2 = H, halo, OH, alkyl, aminoalkyl, CO2H, amino, etc.; R3 = Ph optionally substituted in position 2 by C1-2 alkyl or alkoxy; R4 = F, OH; R5 = H; or R4 = R5 = OH; or R4R5 = bond] and their stereoisomers, isomer mixts., and salts, are claimed (40 synthetic examples). For example, N-acylation of [3a(S),4(S),7a(S)]-7,7-diphenyl-4-(2-methoxyphenyl)perhydroisoindol-4-ol (prepared in 4 steps) with (S)-2-(MeO)C6H4CHMeCO2H (prepared in 3 steps) using EDCI in CH2Cl2 gave title compound II. The ED50 of II for inhibition of increased capillary permeability induced by septide (a substance P agonist) in guinea pigs was 0.04 mg/kg i.v. or 3.5 mg/kg p.o. II also countered hypotension and bronchoconstriction induced by substance P in guinea pigs.
IT 153438-63-2P 153438-64-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as substance P antagonist)
RN 153438-63-2 CAPLUS
CN 1H-Isoindol-4-ol, 2-[(5-fluoro-1H-indol-3-yl)acetyl]octahydro-4-(2-methoxyphenyl)-7,7-diphenyl-, [3aS-(3aα,4β,7aα)]- (9CI) (CA INDEX NAME)

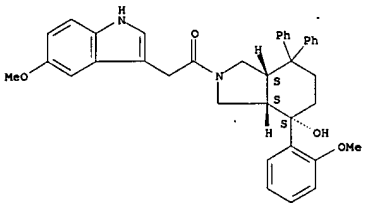
Absolute stereochemistry.



RN 153438-64-3 CAPLUS

L3 ANSWER 48 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
CN 1H-Isoindol-4-ol, octahydro-2-[(5-methoxy-1H-indol-3-yl)acetyl]-4-(2-methoxyphenyl)-7,7-diphenyl-, [3aS-(3aα,4β,7aα)]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

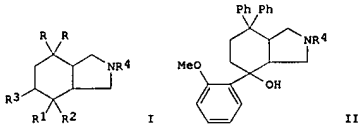


L3 ANSWER 49 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1994:244664 CAPLUS
DOCUMENT NUMBER: 120:244664
TITLE: Preparation of perhydroisoindoles as substance P antagonists
INVENTOR(S): Achard, Daniel; Grisoni, Serge; Malleron, Jean Luc; Peyronel, Jean Francois; Tabart, Michel
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer S.A., Fr.
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9321154	A1	19931028	WO 1993-FR351	19930408
W: AU, CA, CZ, FI, HU, JP, KR, NO, NZ, PL, RU, SK, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
FR 2689889	A1	19931015	FR 1992-4391	19920410
FR 2689889	B1	19940610		
IL 105256	A	19970814	IL 1997-105256	19930401
ZA 9302528	A	19931028	ZA 1993-2528	19930408
AU 9339564	A	19931118	AU 1993-39564	19930408
AU 667365	B2	19960321		
EP 635002	A1	19950125	EP 1993-909004	19930408
EP 635002	B1	19980722		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
JP 07505409	T	19950615	JP 1993-518040	19930408
HU 71330	A2	19951128	HU 1994-2912	19930408
PL 172753	B1	19971128	PL 1993-305359	19930408
AT 168674	T	19980815	AT 1993-909004	19930408
ES 2118954	T3	19981001	ES 1993-909004	19930408
RU 2120438	C1	19981020	RU 1994-45867	19930408
CZ 284596	B6	19990113	CZ 1994-2483	19930408
NO 9403738	A	19941005	NO 1994-3738	19941005
FI 9404728	A	19941007	FI 1994-4728	19941007
FI 105022	B1	20000531		
US 5463077	A	19951031	US 1994-313120	19941011
PRIORITY APPLN. INFO.:			FR 1992-4391 A	19920410
			WO 1993-FR351 A	19930408

OTHER SOURCE(S): MARPAT 120:244664
GI

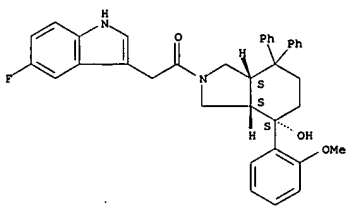
L3 ANSWER 49 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



I II

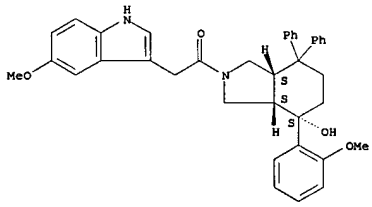
AB Title compds. (I; R = Ph, 2- or 3-halophenyl, -methylphenyl; R1 = Ph, 2-methyl- or -ethylphenyl, -methoxy- or -ethoxyphenyl; R2 = F, OH; R3 = H, OH; R2R3 = bond; R4 = H, protective group) were prepared Thus, (3aRS,7aRS)-7,7-diphenylperhydroisoindol-4-one was converted in 3 steps to (S,S)-I (R = Ph, R1R2 = O, R3 = H, R4 = CO2CMe3) which was condensed with the Grignard reagent from 2-(MeO)C6H4Br to give, after deprotection, isoindolol II (R4 = H). The latter was condensed with (S)-2-(MeO)C6H4CHMeCO2H (preparation given) to give II [R4 = (S)-2-(MeO)C6H4CHMeCO] which had ED50 of 0.7mg/kg i.v. against [pro9] substance P-induced bronchospasm in monkeys.
IT 153438-63-2P 153438-64-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as substance P antagonist)
RN 153438-63-2 CAPLUS
CN 1H-Isoindol-4-ol, 2-[(5-fluoro-1H-indol-3-yl)acetyl]octahydro-4-(2-methoxyphenyl)-7,7-diphenyl-, [3aS-(3aα,4β,7aα)]- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.



RN 153438-64-3 CAPLUS
CN 1H-Isoindol-4-ol, octahydro-2-[(5-methoxy-1H-indol-3-yl)acetyl]-4-(2-methoxyphenyl)-7,7-diphenyl-, [3aS-(3aα,4β,7aα)]- (9CI)
(CA INDEX NAME)

L3 ANSWER 49 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
Absolute stereochemistry.

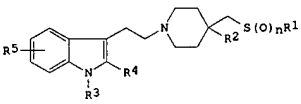


L3 ANSWER 50 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:671015 CAPLUS
DOCUMENT NUMBER: 119:271015
TITLE: (Indolylethyl)piperidine NK2 receptor antagonists
INVENTOR(S): Cooper, Anthony William James; Hagan, Russell Michael
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9314084	A2	19930722	WO 1993-EP101	19930115
WO 9314084	A3	19931014		
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9333513	A	19930803	AU 1993-33513	19930115

PRIORITY APPLN. INFO.: GB 1992-1179 A 19920121
WO 1993-EP101 A 19930115

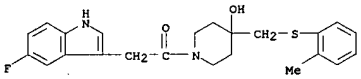
OTHER SOURCE(S): MARPAT 119:271015
GI



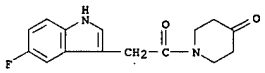
I

AB The title compds. I [R1 = (un)substituted Ph; R2 = H, HO, C1-4 alkoxy; R3 = H, C1-4 alkyl; R4 = H, C1-4 alkyl, C1-4 alkoxy; R5 = H, C1-4 alkyl, CF3, CN, halogen; n = 0-2], useful in the treatment of conditions mediated by tachykinins, including NKA, NKB, and substance P, acting at the NK2 receptor, are prepared Thus, (R)-methylphenyl sulfoxide was reacted with Li bis(trimethylsilyl)amide, and the intermediate reacted with 1-[5-fluoro-1H-indol-3-yl)ethyl]-4-piperidone, followed by methanesulfonic acid, producing (R)-1-[2-(5-fluoro-1H-indol-3-yl)ethyl]-4-[(phenylsulfinyl)methyl]-4-piperidinol methanesulfonic acid salt (II). II demonstrated anxiolytic activity in the mouse light-dark box and the rat elevated plus-maze.
IT 151191-69-4P 151191-70-7P 151191-71-8P
151191-75-2P 151191-78-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

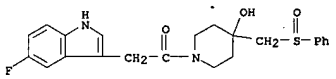
L3 ANSWER 50 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



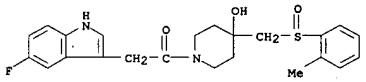
L3 ANSWER 50 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(Reactant or reagent)
(prepn. and reaction of, in prepn. of NK2 receptor antagonists)
RN 151191-69-4 CAPLUS
CN 4-Piperidinone, 1-[(5-fluoro-1H-indol-3-yl)acetyl]- (9CI) (CA INDEX NAME)



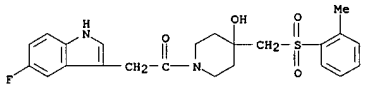
RN 151191-70-7 CAPLUS
CN 4-Piperidinol, 1-[(5-fluoro-1H-indol-3-yl)acetyl]-4-[(phenylsulfinyl)methyl]- (9CI) (CA INDEX NAME)



RN 151191-71-8 CAPLUS
CN 4-Piperidinol, 1-[(5-fluoro-1H-indol-3-yl)acetyl]-4-[[(2-methylphenyl)sulfinyl]methyl]- (9CI) (CA INDEX NAME)

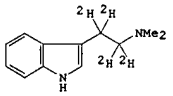


RN 151191-75-2 CAPLUS
CN 4-Piperidinol, 1-[(5-fluoro-1H-indol-3-yl)acetyl]-4-[[(2-methylphenyl)sulfonyl]methyl]- (9CI) (CA INDEX NAME)



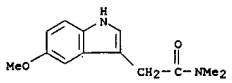
RN 151191-78-5 CAPLUS
CN 4-Piperidinol, 1-[(5-fluoro-1H-indol-3-yl)acetyl]-4-[[(2-methylphenyl)thio]methyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 51 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:670946 CAPLUS
DOCUMENT NUMBER: 119:270946
TITLE: Indolealkylamine metabolism: synthesis of deuterated indolealkylamines as metabolic probes
AUTHOR(S): Morris, Philip E., Jr.; Chiao, Cheng
CORPORATE SOURCE: Dep. Chem., Univ. Alabama, Birmingham, AL, 35294, USA
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals
(1993), 33(6), 455-65
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:270946
GI



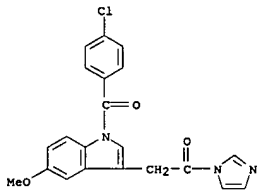
I

AB The synthesis of the deuterium labeled, endogenously occurring, indolealkylamine hallucinogens N,N-dimethyltryptamine and 5-methoxy-N,N-dimethyltryptamine via reduction of amide intermediates with lithium aluminum deuteride (LAD) is described. Thus, 2-(3-indolyl)glyoxal chloride was treated with Me2NH to give 2-(3-indolyl)-N,N-dimethylglyoxalamide which was reduced with LAD to give α,α,β,β-[2H]4-N,N-dimethyltryptamine (I). The compds. were characterized with 1H, 2H and 13C NMR. These compds. were synthesized for use as probes for investigating the metabolism of these compds. by MAO via the in vivo kinetic isotope effect.
IT 151290-19-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 151290-19-6 CAPLUS
CN 1H-Indole-3-acetamide, 5-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

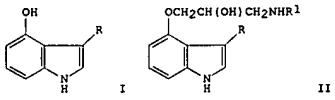


L3 ANSWER 52 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:440466 CAPLUS
DOCUMENT NUMBER: 119:40466
TITLE: Inactivation of prostaglandin endoperoxide synthase by acylating derivatives of indomethacin
AUTHOR(S): Wells, Isabelle; Marnett, Lawrence J.
CORPORATE SOURCE: Sch. Med., Vanderbilt Univ., Nashville, TN, 37232-0146, USA
SOURCE: Biochemistry (1993), 32(10), 2710-16
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Derivs. of the potent antiinflammatory agent and cyclooxygenase inhibitor indomethacin were synthesized in which the carboxylic acid moiety was converted into reactive acylating agents. Indomethacin imidazole (indomethacin-IM) and indomethacin N-hydroxysuccinimide (indomethacin-NHS) inactivated both the cyclooxygenase and peroxidase activities when incubated with the apo form of purified prostaglandin endoperoxide synthase (PGH synthase) at a stoichiometry of 1:1. Treatment of the inactivated enzyme with hydroxylamine at neutral pH led to recovery of all peroxidase and about 50% of the cyclooxygenase activity. Hydroxylamine did not regenerate the cyclooxygenase activity of the indomethacin-inactivated protein. Reconstitution of the apoprotein with heme protected against inactivation by indomethacin-NHS. Visible spectroscopy established that indomethacin-NHS-inactivated apoenzyme had a reduced capacity to bind heme. Indomethacin-NHS also substantially protected the apoenzyme from cleavage at the trypsin-sensitive Arg277 site. Incubation of [2-14C]indomethacin-NHS with PGH synthase led to incorporation of radioactivity into the protein, but no adduct was detected by reversed-phase HPLC, suggesting it was unstable to the chromatog. conditions. Incubation of indomethacin-NHS with apoprotein followed by HPLC anal. led to the formation of greater amts. of the hydrolysis product indomethacin than did similar treatment of holoprotein. The results suggest that indomethacin-IM and indomethacin-NHS covalently and selectively label PGH synthase near the heme binding site, leading to loss of both catalytic activities of the enzyme.
IT 148560-94-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and prostaglandin endoperoxide synthase cyclooxygenase and peroxidase activity inactivation by)
RN 148560-94-5 CAPLUS
CN 1H-Indole, 1-(4-chlorobenzoyl)-3-[2-(1H-imidazol-1-yl)-2-oxoethyl]-5-methoxy- (9CI) (CA INDEX NAME)

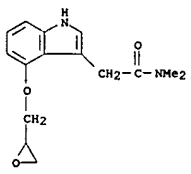
L3 ANSWER 52 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L3 ANSWER 53 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:168924 CAPLUS
DOCUMENT NUMBER: 118:168924
TITLE: Search for β-adrenoblockers among aminooxypropyl derivatives of 4-hydroxyindolylacetic acid and 4-hydroxyskatole
AUTHOR(S): Glushkov, R. G.; Mashkovskii, M. D.; Skryabin, G. K.; Suvorov, N. N.; Kozlovskii, A. G.; Vinograd, L. Kh.; Yuzhakov, S. D.; Arinbasarov, M. U.; Tribunskaya, Yu. I.; et al.
CORPORATE SOURCE: TSKhLS, VNIKhFI im. S. Ordzhonikidze, Moscow, Russia
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1992), 26(6), 18-21
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 118:168924
GI

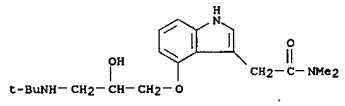


AB Treating indoles I (R = CH2CO2Me, Me, CH2CONH2, CH2CONMe2) with 2-(chloromethyl)oxirane gave 74-82.5% glycidyloxy derivs. which were substituted by Me2CHNH2 and Me3CNH2 to give 60.5-94.5% aminohydroxypropoxy derivs. II (R1 = Me2CH, CMe3). The highest blocking activity was displayed by II (R = Me, R1 = CMe3) and by II (R = CH2CO2Me, R1 = CMe3).
IT 145101-56-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and amination by isopropyl- and tert-butylamines)
RN 145101-56-0 CAPLUS
CN 1H-Indole-3-acetamide, N,N-dimethyl-4-(oxiranylmethoxy)- (9CI) (CA INDEX NAME)

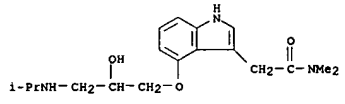


IT 145101-61-7P
RL: SPN (Synthetic preparation); PREP (Preparation)

L3 ANSWER 53 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(prepn. and condensation with acetone)
RN 145101-61-7 CAPLUS
CN 1H-Indole-3-acetamide, 4-[3-[(1,1-dimethylethyl)amino]-2-hydroxypropoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)



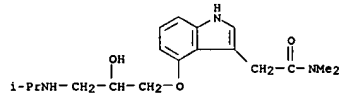
IT 145101-60-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and β-adrenergic antagonist activity of)
RN 145101-60-6 CAPLUS
CN 1H-Indole-3-acetamide, 4-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]-N,N-dimethyl- (9CI) (CA INDEX NAME)



IT 145296-55-5P 145296-56-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 145296-55-5 CAPLUS
CN 1H-Indole-3-acetamide, 4-[2-hydroxy-3-[(1-methylethyl)amino]propoxy]-N,N-dimethyl-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 145101-60-6
CMF C18 H27 N3 O3

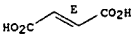


CM 2

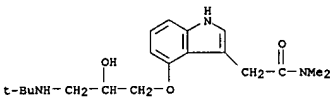
CRN 110-17-8
CMF C4 H4 O4

L3 ANSWER 53 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

Double bond geometry as shown.

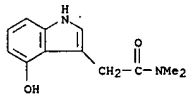


RN 145296-56-6 CAPLUS
CN 1H-Indole-3-acetamide, 4-[3-[(1,1-dimethylethyl)amino]-2-hydroxypropoxy]-N,N-dimethyl-, dihydrochloride (9CI) (CA INDEX NAME)

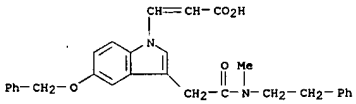


●2 HCl

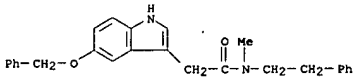
IT 145101-52-6
RL: PROC (Process)
(substitution of, by epichlorohydrin)
RN 145101-52-6 CAPLUS
CN 1H-Indole-3-acetamide, 4-hydroxy-N,N-dimethyl- (9CI) (CA INDEX NAME)



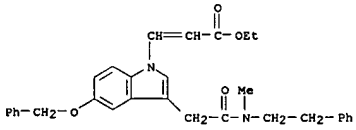
L3 ANSWER 54 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
RN 141835-21-4 CAPLUS
CN 2-Propenoic acid, 3-[3-[2-[methyl(2-phenylethyl)amino]-2-oxoethyl]-5-(phenylmethoxy)-1H-indol-1-yl]- (9CI) (CA INDEX NAME)



IT 141835-68-9P 141835-69-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate in preparation of LTB4 antagonist)
RN 141835-68-9 CAPLUS
CN 1H-Indole-3-acetamide, N-methyl-N-(2-phenylethyl)-5-(phenylmethoxy)-(9CI)
(CA INDEX NAME)



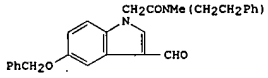
RN 141835-69-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[2-[methyl(2-phenylethyl)amino]-2-oxoethyl]-5-(phenylmethoxy)-1H-indol-1-yl]-, ethyl ester (9CI) (CA INDEX NAME)



L3 ANSWER 54 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1992:448333 CAPLUS
DOCUMENT NUMBER: 117:48333
TITLE: Preparation of substituted bicyclic arylindole compounds exhibiting selective leukotriene B4 antagonist activity
INVENTOR(S): Huang, Fu Chih; Chan, Wan K.; Sutherland, Charles A.; Galemmo, Robert A., Jr.
PATENT ASSIGNEE(S): Rhone-Poulenc Rorer International (Holdings), Inc., USA
SOURCE: PCT Int. Appl., 87 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9204321	A1	19920319	WO 1991-US6447	19910906
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
CA 2091257	A1	19920311	CA 1991-2091257	19910906
AU 9186419	A	19920330	AU 1991-86419	19910906
EP 548250	A1	19930630	EP 1991-917468	19910906
EP 548250	B1	19960327		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 06504520	T	19940526	JP 1991-516161	19910906
JP 3334087	B2	20021015		
AT 136026	T	19960415	AT 1991-917468	19910906
US 5468898	A	19951121	US 1993-777246	19930423
PRIORITY APPLN. INFO.:			US 1990-580243	A2 19900910
			WO 1991-US6447	A 19910906

OTHER SOURCE(S): MARPAT 117:48333
GI



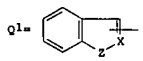
I

AB The title compds., useful as leukotriene B4 antagonists for treatment of disorders which result from LTB4 activity (no data), are prepared To NaH in THF, 5-(benzyloxy)indole-3-carboxaldehyde (preparation given) was added, followed by BrCH2CON(CH2CH2Ph)Me, to give the title indole I. Addnl. title compds. were prepared
IT 141835-21-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as LTB4 antagonist)

L3 ANSWER 55 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:82562 CAPLUS
DOCUMENT NUMBER: 114:82562
TITLE: Preparation of acyldipeptide amides as tachykinin antagonists
INVENTOR(S): Matsuo, Masaaki; Hagiwara, Daijiro; Miyake, Hiroshi
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 13 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 394989	A2	19901031	EP 1990-107822	19900425
EP 394989	A3	19910424		
EP 394989	B1	19941221		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 5164372	A	19921117	US 1990-505457	19900406
CA 2015359	A1	19901028	CA 1990-2015359	19900425
JP 03027399	A	19910205	JP 1990-114129	19900427
PRIORITY APPLN. INFO.:			GB 1989-9795	A 19890428
			GB 1989-17542	A 19890801

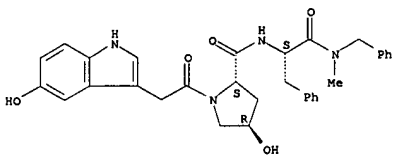
OTHER SOURCE(S): MARPAT 114:82562
GI



AB R1YCOANR2CH(CH2C6H4R3-p)CONR4R5 [R1 = (substituted) alkyl, aryl, arylamino, pyridyl, pyrrolyl, pyrazolopyridyl, quinolyl, Q1; X = CH, N; Z = O, S, NH; R2 = H, alkyl; R3 = H, OH; R4 = (substituted) alkyl; R5 = pyridylalkyl, (substituted) aralkyl; or R4R5 = benzene-condensed alkylene; A = amino acid residue except D-Trp; Y = bond, alkylene, alkenylene], were prepared Thus, BOC-Q2-Phe-N(Me)CH2Ph [BOC = Me3CO2C, Q2 = (2S,4R)-4-hydroxylprolyl residue] (preparation from BOC-Phe-OH given) was deprotected with trifluoroacetic acid and the product was coupled with indole-3-carbonyl chloride (Q3Cl) in CH2Cl2 in the presence of bistrimethylsilylacetamide to give Q3-Q2-Phe-N(Me)CH2Ph. The latter inhibited substance P-induced bronchoconstriction in guinea pigs with an ED50 of 0.072 mg/kg intratracheally.
IT 131948-37-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as tachykinin antagonist)
RN 131948-37-3 CAPLUS
CN L-Phenylalaninamide, [illegible]-1H-indol-3-yl)acetyl]-L-

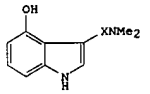
L3 ANSWER 55 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
prolyl-N-methyl-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L3 ANSWER 56 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1986:552787 CAPLUS
DOCUMENT NUMBER: 105:152787
TITLE: Synthesis of psilocin labeled with carbon-14 and tritium
AUTHOR(S): Poon, Grace; Chui, Yun Cheung; Law, Francis C. P.
CORPORATE SOURCE: Dep. Biol. Sci., Simon Fraser Univ., Burnaby, BC, V5A 1S6, Can.
SOURCE: Journal of Labelled Compounds and Radiopharmaceuticals
(1986), 23(2), 167-74
CODEN: JLCRD4; ISSN: 0362-4803
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:152787
GI



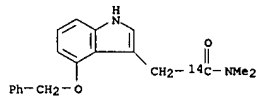
I

AB 14C- and 3H-labeled psilocin (I, X = CH214CH2; C3H2C3H2) tryptamine), the principal active agent of hallucinogenic mushrooms, was synthesized from 2-methyl-3-nitrophenol via 4-benzyloxyindole. 4-Benzyloxygramine was treated with K14CN to give 14C-4-benzyloxy-3-indoleacetic acid, an intermediate for I (X = CH214CH2). LiAl3H4 was used to reduce 4-benzyloxy-3-indole-N,N-dimethylglyoxylamide to give I (X = C3H2C3H2).

IT 104556-01-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 104556-01-6 CAPLUS

CN 1H-Indole-3-acetamide-carbonyl-14C, N,N-dimethyl-4-(phenylmethoxy)- (9CI) (CA INDEX NAME)



L3 ANSWER 57 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

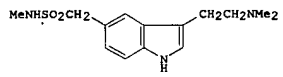
ACCESSION NUMBER: 1986:478831 CAPLUS
DOCUMENT NUMBER: 105:78831
TITLE: 3-[2-(Dimethylamino)ethyl]-N-methyl-1H-indole-5-methanesulfonamide
INVENTOR(S): Oxford, Alexander William
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Ger. Offen., 57 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3527648	A1	19860213	DE 1985-3527648	19850801
DE 3527648	C2	19930826		
CH 666026	A5	19880630	CH 1985-3296	19850730
HU 40077	A2	19861128	HU 1985-2945	19850731
HU 201738	B	19901228		
DK 8503511	A	19860202	DK 1985-3511	19850801
DK 158942	B	19900806		
DK 158942	C	19910121		
FI 8502969	A	19860202	FI 1985-2969	19850801
FI 78466	B	19890428		
FI 78466	C	19890810		
SE 8503680	A	19860202	SE 1985-3680	19850801
SE 452460	B	19871130		
SE 452460	C	19880310		
BE 903006	A1	19860203	BE 1985-215426	19850801
NO 8503046	A	19860203	NO 1985-3046	19850801
NO 164653	B	19900723		
NO 164653	C	19901107		
GB 2162522	A	19860205	GB 1985-19418	19850801
GB 2162522	B	19880224		
AU 8545689	A	19860206	AU 1985-45689	19850801
AU 573878	B2	19880623		
FR 2568571	A1	19860207	FR 1985-11790	19850801
FR 2568571	B1	19880923		
NL 8502171	A	19860303	NL 1985-2171	19850801
NL 188642	B	19920316		
NL 188642	C	19920817		
JP 61047464	A	19860307	JP 1985-168664	19850801
JP 06023197	B	19940330		
ZA 8505818	A	19860430	ZA 1985-5818	19850801
ES 545810	A1	19861016	ES 1985-545810	19850801
AT 8502266	A	19871215	AT 1985-2266	19850801
AT 386196	B	19880711		
CA 1241004	A1	19880823	CA 1985-487992	19850801
PL 146005	B1	19881231	PL 1985-254800	19850801
IL 75986	A	19890228	IL 1985-75986	19850801
SU 1498386	A3	19890730	SU 1985-3935745	19850801
ES 552047	A1	19871216	ES 1986-552047	19860214
ES 557480	A1	19880216	ES 1987-557480	19870331
ES 557481	A1	19880216	ES 1987-557481	19870331
ES 557483	A1	19880216	ES 1987-557483	19870331
ES 557482	A1	19880301	ES 1987-557482	19870331
US 5037845	A	19910806	US 1989-317682	19890301
SK 277952	B6	19950913	SK 1991-4041	19911223

L3 ANSWER 57 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

CZ 280530	B6	19960214	CZ 1991-4041	19911223
PRIORITY APPLN. INFO.:			GB 1984-19575 A	19840801
			US 1985-761392 B1	19850801
			US 1987-82666 B1	19870807

OTHER SOURCE(S): CASREACT 105:78831
GI



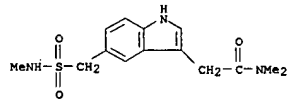
I

AB The title compound (I), prepared by 8 methods, is useful in treating migraine headaches at 0.1-100 mg per dose, up to 8 times daily. Hydrogenation of 3-(cyanomethyl)-N-methyl-1H-indole-5-methanesulfonamide over prereduced 10% Pd oxide on active C in methanolic and ethanolic Me2NH for 24 h at room temperature gave I (isolated as the succinate). Several formulations were given.

IT 103628-52-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of)

RN 103628-52-0 CAPLUS

CN 1H-Indole-3-acetamide, N,N-dimethyl-5-[[(methylamino)sulfonyl]methyl]- (9CI) (CA INDEX NAME)



L3 ANSWER 58 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

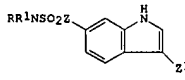
ACCESSION NUMBER: 1985:560388 CAPLUS
DOCUMENT NUMBER: 103:160388
TITLE: Indole derivatives and their use
INVENTOR(S): Oxford, Alexander William; Evans, Brian; Dowle, Michael Dennis; Coates, Ian Harold
PATENT ASSIGNEE(S): Glaxo Group Ltd., UK
SOURCE: Ger. Offen., 72 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3444572	A1	19850620	DE 1984-3444572	19841206
DE 3444572	C2	19931014		
FI 8404789	A	19850607	FI 1984-4789	19841205
FI 80260	B	19900131		
FI 80260	C	19900510		
BE 901224	A1	19850606	BE 1984-214125	19841206
DK 8405836	A	19850607	DK 1984-5836	19841206
FR 2555987	A1	19850607	FR 1984-18618	19841206
FR 2555987	B1	19870717		
NO 8404879	A	19850607	NO 1984-4879	19841206
NO 162764	B	19891106		
NO 162764	C	19900214		
SE 8406200	A	19850607	SE 1984-6200	19841206
SE 458446	B	19890403		
SE 458446	C	19890727		
AU 8436367	A	19850613	AU 1984-36367	19841206
AU 575365	B2	19880728		
NL 8403719	A	19850701	NL 1984-3719	19841206
GB 2150932	A	19850710	GB 1984-30810	19841206
GB 2150932	B	19871028		
JP 60155156	A	19850815	JP 1984-258409	19841206
JP 06002733	B	19940112		
AT 8403873	A	19860515	AT 1984-3873	19841206
AT 381934	B	19861210		
ES 538336	A1	19860601	ES 1984-538336	19841206
ZA 8409498	A	19860924	ZA 1984-9498	19841206
CH 663411	A5	19871215	CH 1984-5810	19841206
CA 1233183	A1	19880223	CA 1984-469528	19841206
IL 73756	A	19880229	IL 1984-73756	19841206
HU 40624	A2	19870128	HU 1985-2083	19850530
CN 85104233	A	19870107	CN 1985-104233	19850603
CN 85106225	A	19870218	CN 1985-106225	19850819
CN 1015055	B	19911211		
ES 546631	A1	19871016	ES 1985-546631	19850902
US 4994483	A	19910219	US 1989-443874	19891130
DK 9002140	A	19900906	DK 1990-2140	19900906
JP 03184958	A	19910812	JP 1990-326200	19901129

PRIORITY APPLN. INFO.: GB 1983-32435 A 19831206
US 1984-678995 B1 19841206

L3 ANSWER 58 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
US 1987-72786 B1 19870713

OTHER SOURCE(S): CASREACT 103:160388; MARPAT 103:160388
GI

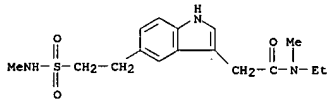


I

AB Antimigraine (no data) indolealkanesulfonamides I [R = H, alkyl, alkenyl; R1 = cycloalkyl, Ph, phenylalkyl, R; R2, R3 = H, alkyl, CH2:CHCH2; R2R3 = aralkylidene; Z, Z1 = alkyl-(un)substituted alkylene] were prepared Thus, 4-O2NC6H4CH2CH2SO2Cl was amidated with MeNH2, hydrogenated over Pd-C to the aniline, diazotized, and treated with ZnCl2 to give 4-H2NNHC6H4CH2CH2SO2NHMe. The latter compound was stirred in aqueous MeOH with (MeO)2CH(CH2)3Cl at 50°, NH4OAc added to pH 4, then refluxed 5 h to give I (R = Me, R1-R3 = H, Z = Z1 = CH2CH2).

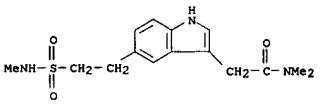
IT 98622-74-3P 98623-48-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and lithium aluminum hydride reduction of)

RN 98622-74-3 CAPLUS
CN 1H-Indole-3-acetamide, N-ethyl-N-methyl-5-[2-[(methylamino)sulfonyl]ethyl]- (9CI) (CA INDEX NAME)



RN 98623-48-4 CAPLUS
CN 1H-Indole-3-acetamide, N,N-dimethyl-5-[2-[(methylamino)sulfonyl]ethyl]- (9CI) (CA INDEX NAME)

L3 ANSWER 58 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



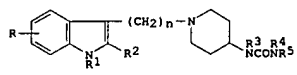
L3 ANSWER 59 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1977:16538 CAPLUS
DOCUMENT NUMBER: 86:16538
TITLE: Indolylalkylpiperidines
INVENTOR(S): Huebner, Charles F.
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Ger. Offen., 72 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2609289	A1	19760930	DE 1976-2609289	19760306
SE 7602729	A	19760913	SE 1976-2729	19760227
NO 7600774	A	19760913	NO 1976-774	19760305
GB 1534351	A	19781206	GB 1976-8902	19760305
FI 7600584	A	19760911	FI 1976-584	19760308
FR 2303541	A1	19761008	FR 1976-6495	19760308
FR 2303541	B1	19791005		
ES 445874	A1	19770601	ES 1976-445874	19760308
AU 7611750	A	19770915	AU 1976-11750	19760308
IL 49171	A	19781217	IL 1976-49171	19760308
BE 839347	A1	19760909	BE 1976-164977	19760309
DK 7601014	A	19760911	DK 1976-1014	19760309
DK 138893	C	19790423		
DK 138893	B	19781113		
DD 124386	A5	19770216	DD 1976-191763	19760309
NL 7602508	A	19760914	NL 1976-2508	19760310
JP 51113878	A	19761007	JP 1976-26622	19760310
US 4147786	A	19790403	US 1977-797151	19770516
US 4242347	A	19801230	US 1979-50003	19790618

PRIORITY APPLN. INFO.: US 1975-556600 A 19750310
US 1976-654254 A3 19760202

OTHER SOURCE(S): CASREACT 86:16538
GI

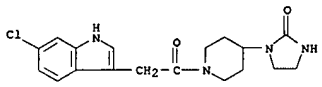


I

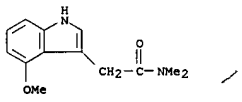
AB Indolylethylpiperidines (I; R = e.g., H, 5-Cl, 5-Br, 5-F, 7-Me, 7-MeO; R1 = e.g., H, Me; R2 = e.g., H, Me; R3, R4 = e.g., H, H; ethylene, o-phenylene; R5 = e.g., H, Ph; n = 2, 3), useful as antihypertensives, are prepared by various known procedures. Thus, reaction of 3-(2-bromoethyl)indole with 4-ureidopiperidine in DMF 2 days at room temperature in presence of Et3N gives I (R = R1 = R2 = R3 = R4 = R5 = H, n = 2).

IT 61220-26-6P
RL: BAC (Biological activity or effector, except adverse); BSU

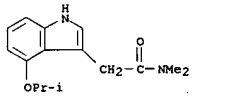
L3 ANSWER 59 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and antihypertensive activity of)
RN 61220-26-6 CAPLUS
CN Piperidine, 1-[(6-chloro-1H-indol-3-yl)acetyl]-4-(2-oxo-1-imidazolidinyl)- (9CI) (CA INDEX NAME)



L3 ANSWER 60 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1974:145952 CAPLUS
DOCUMENT NUMBER: 80:145952
TITLE: New route for synthesizing psilocine derivatives
AUTHOR(S): Germain, Claude; Bourdais, Jacques
CORPORATE SOURCE: Lab. Chim. Heterocyclique Organomet., Univ. Paris-Sud, Orsay, Fr.
SOURCE: Chimica Therapeutica (1973), 8(6), 647-51
CODEN: CHTPBA; ISSN: 0009-4374
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 80:145952
GI For diagram(s), see printed CA Issue.
AB Indoles I (R = Me, PhCH2; R1 = Me, Me2CH n = 1.2) were prepared from 2,3-Cl(O2N)C6H3OH (II). Successive methylation, NCCH2CONMe2 condensation, hydrogenation and reductive cyclization of II indolecarboxamide III (R = H, R1 = Me, m = 0), which underwent alkylation and LiAlH4 reduction to give indolemethylamines I (R = PhCH2, 2-ClC6H4CH2). In 6 steps III (R = H, R1 = Me, m = 0) was converted to the indoleacetamide III (m = 1), which was reduced to the corresponding indoleethylamine I. Alkylation of III (R = H, R1 = Me, m = 1) and then reduction gave indoleethylamine I (R = Me, PhCH2). Similarly, I (R1 = Me2CH) were prepared
IT 52335-79-2P 52335-80-5P 52335-81-6P 52335-82-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 52335-79-2 CAPLUS
CN 1H-Indole-3-acetamide, 4-methoxy-N,N-dimethyl- (9CI) (CA INDEX NAME)

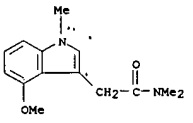


RN 52335-80-5 CAPLUS
CN 1H-Indole-3-acetamide, N,N-dimethyl-4-(1-methylethoxy)- (9CI) (CA INDEX NAME)



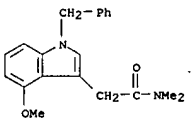
L3 ANSWER 60 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

RN 52335-81-6 CAPLUS
CN 1H-Indole-3-acetamide, 4-methoxy-N,N,1-trimethyl- (9CI) (CA INDEX NAME)



4-methoxy

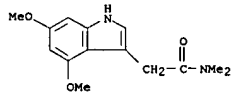
RN 52335-82-7 CAPLUS
CN 1H-Indole-3-acetamide, 4-methoxy-N,N-dimethyl-1-(phenylmethyl)- (9CI) (CA INDEX NAME)



R2 = alkyl

Brown (892)

L3 ANSWER 61 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1969:491200 CAPLUS
DOCUMENT NUMBER: 71:91200
TITLE: Synthesis and reactions of 4,6-dimethoxyindole, and unusual indole system
AUTHOR(S): Brown, Vernon H.; Skinner, W. A.; DeGraw, Joseph I.
CORPORATE SOURCE: Dep. of Pharm. Chem., Stanford Res. Inst., Menlo Park, CA, USA
SOURCE: Journal of Heterocyclic Chemistry (1969), 6(4), 539-43
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 71:91200
GI For diagram(s), see printed CA Issue.
AB A synthesis of 4,6-dimethoxyindole (I) is described. Formylation or oxalylation reactions with I gave substitution at position 7 rather than the usual 3-substitution characteristic of other indoles. A synthesis of N,N-dimethyl-4,6-dimethoxytryptamine is presented along with N.M.R. data for 3 and 7-substituted compds. in this series.
IT 23659-97-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23659-97-4 CAPLUS
CN Indole-3-acetamide, 4,6-dimethoxy-N,N-dimethyl- (8CI) (CA INDEX NAME)

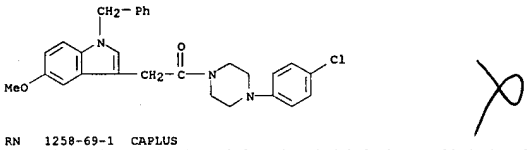


L3 ANSWER 62 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1965:36828 CAPLUS
DOCUMENT NUMBER: 62:36828
ORIGINAL REFERENCE NO.: 62:6485a-c
TITLE: Synthesis of some N-phenylpiperazine derivatives as potential central nervous system depressants
AUTHOR(S): Chou, Chi-Ting; Chi, Ju-Yun
CORPORATE SOURCE: Acad. Sinica, Shanghai, Peop. Rep. China
SOURCE: Yaoxue Xuebao (1964), 11(10), 692-9
CODEN: YHHPAL; ISSN: 0513-4870
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB A series of indolylalkylphenylpiperazines was recently reported to be active central nervous system depressants. Variation in the length of the alkyl chains and change of substituents on the indole moiety or on the Ph group influenced only the strength and specificity of the activity. However, removal of the Ph group or replacement of it by an alkyl or arylalkyl group caused the loss of almost all of the central activities. It would seem possible to get even more favorable central nervous system depressants on further modification of the indole moiety, as long as the N-Ph group was retained. A number of N-phenyl- and -chlorophenylpiperazine derivs., the substituents on the other N being either isosteres of indole or pharmacol. interesting groups, were synthesized. These compds. were synthesized either by condensation of appropriate halides with N-phenyl-or-chlorophenylpiperazine, or by reduction of the corresponding amides by means of LiAlH4. The amides were in turn prepared by the interaction of acyl chlorides or acyl azides and N-phenyl- or -chlorophenylpiperazine, resp. Two of the amides were afforded on application of the Arndt-Eistert reaction. Two of these compds., 1-(3,4,5-trimethoxyphenethyl)-4-phenylpiperazine and 1-(3,4,5-trimethoxyphenethyl)-4-(p-chlorophenyl)piperazine exhibited marked tranquilizing activity in preliminary pharmacol. examns.

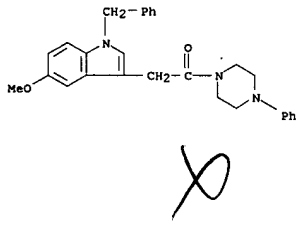
IT 1109-25-7P, Piperazine, 1-[(1-benzyl-5-methoxyindol-3-yl)acetyl]-4-(p-chlorophenyl)- 1258-69-1P, Piperazine, 1-[(1-benzyl-5-methoxyindol-3-yl)acetyl]-4-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 1109-25-7 CAPLUS
CN Piperazine, 1-[(1-benzyl-5-methoxyindol-3-yl)acetyl]-4-(p-chlorophenyl)- (7CI, 8CI) (CA INDEX NAME)



RN 1258-69-1 CAPLUS
CN Piperazine, 1-[(1-benzyl-5-methoxyindol-3-yl)acetyl]-4-phenyl- (7CI, 8CI)

L3 ANSWER 62 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
(CA INDEX NAME)



L3 ANSWER 63 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1964:52796 CAPLUS
DOCUMENT NUMBER: 60:52796
ORIGINAL REFERENCE NO.: 60:9293g-h,9294a-h,9295a-h,9296a-b
TITLE: Indolylpiperazines
PATENT ASSIGNEE(S): Sterling Drug Inc.
SOURCE: 41 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 944443		19631211	GB	
US 3188313		19650608	US 1959-842203	19590925
PRIORITY APPLN. INFO.:			US	19590925

GI For diagram(s), see printed CA Issue.

AB Compds. of type I and II, in which R1 is H, halogen, alkyl, alkoxy, or aryl, R2 is H, alkyl, hydroxyalkyl, or aryl, R3 and R4 is H, alkyl, or aryl, n is 1 to 7, and in which the indole group may be joined in the 2-position or (as shown) the 3-position, were made. These are useful as hypotensive agents, as antinauseants, antipyretics, sedatives, tranquilizers and muscle relaxants; they inhibit apomorphine-induced vomiting, and prolong the narcosis of ether and barbiturates. A solution of 177 g. (PhCH2)2NCH2CH2NHPh, 120 g. ClCH2COCl and 650 m. CHCl3 was refluxed for 5.5 hrs. to yield 190 g. (PhCH2)2NCH2CH2NPhCOCH2Cl, an oil. This was dissolved in EtOCH2CH2OH, the solution refluxed 4 hrs., cooled, diluted with 650 ml. absolute EtOH, 4 g. Pd-C added, and the mixture reduced by H at 50 lb./in.2 to give 1-phenyl-2-piperazinone (VI), m. 100-5° (p-toluenesulfonate m. 220.2-4.6°). Similarly made from (PhCH2)2NCH2CH2N(4-ClC6H4)(COCH2Cl) (HCl salt m. 161.0-3.8°) was 1-(4-chlorophenyl)-2-piperazinone (HCl salt m. 192.8-4.8°); from 4-benzyl-1-(2,6-dimethylphenyl)-2-piperazinone (HCl salt m. 248.8-64.8°), 1-(2,6-dimethylphenyl)-2-piperazinone (HCl salt m. 224.8-6.0). The I and II were made by various methods. Method A: A mixture of 5.6 g. 2-(3-indolyl)ethyl bromide (VII), 4.1 g. 1-phenylpiperazine, 2.1 g. NaHCO3, and 30 ml. absolute EtOH was refluxed for 6 hrs. to yield 1.4 g. I (R1 = R3 = R4 = H, R2 = Ph, n = 2), m. 131.6-6.0°. Similarly prepared were these I (R3 = R4 = H, n = 2; R1, R2, and m.p. given): H, 4-ClC6H4, 185.2-6.8°; H, p-tolyl, 147.8-54.8°; 5-MeO, p-tolyl, 108.6-11.0°; H, PhCH:CHCH2, 258.2-63.6°. Also made was 1-[2-(3-indolyl)ethyl]-trans-2,5-dimethylpiperazine, m. 189.2-90.4°, and from VI and VII 1-[2-(3-indolyl)ethyl]-4-phenyl-3-piperazinone, m. 163.2-4.4°. Method B: To a cold solution of 79.2 g. 1-(o-tolyl)piperazine in 500 ml. tetrahydrofuran (VIII) was added 31.2 g. (3-indolyl)glyoxalyl chloride (IX), the white precipitate filtered off, the filtrate evaporated, the residual gum taken up in a warm mixture of 700 ml. H2O, 120 ml. AcOEt and 25 ml. AcOH, and the solid collected, to give 41.5 g. III (R1 = R3 = R4 = H, R2 = o-tolyl) (X). Similarly prepared were these III

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(R3 = R4 = H; R1, R2, and m.p. given): H, Me, --; H, HOCH2CH2, --; H, m-tolyl, --; H, 2-MeOC6H4, --; H, 4-MeOC6H4, 243-5°; H, 3,4-ClMeC6H3, 211-14°; 6-MeO, Ph, 205-9°; 6-MeO, o-tolyl, 247-50°; 6-MeO, m-tolyl, 206-8°; 6-MeO, p-tolyl, 196-8°; 6-MeO, 2-MeOC6H4, 246-8°; 6-MeO, 4-MeOC6H4, 205-10°; 5-PhCH2O, p-tolyl, 148-55°; 5-PhCH2O, PhCH2CH2, 135-40°; 5-MeS, Ph, 188-91°; 5-MeS, p-tolyl, 211-13°; 5,6-(CH2O2), Ph, 267-9°; 5,6-(CH2O2), o-tolyl, 214.6-15.8°; 5,6-(CH2O2), m-tolyl, 212-16°; 5,6-(CH2O2), p-tolyl, 266.4-78.4°; 5,6-(CH2O2), 2-MeOCH2CH2, 205-9°; 5,6-(MeO)2, Ph, 256.8-8.8°; 5,6-(MeO)2, o-tolyl, 211-16°; 5,6-(MeO)2, m-tolyl, 231-8°; 5,6-(MeO)2, p-tolyl, --; 5,6-(MeO)2, 2-MeOC6H4, 218-22°; 5,6-(MeO)2, 3-MeOC6H4, 234.4-6.4°; 5 6-(MeO)2, 4-MeOC6H4, 228-36°; 5,6-(MeO)2, 4-MeSC6H4, 236.4-8.2°; 5,6-(EtO)2, Ph, 180.0-1.0°; H, 2-pyridyl, 242-3°; 4-MeO, Ph, --; 5-MeO, Ph, 224-7.5°; 7-MeO, Ph, --; 6-Me, Ph, --; 6-EtO, Ph, 165° (decompn.); 6-MeO, 2-ClC6H4, 125.2-8.8°; 6-MeO, 3-ClC6H4, 214-16°; 6-MeO, 3-MeOC6H4, 211-13°; 6-MeO, 2-EtOC6H4, 180-4°; 6-MeO, 2,6-Me2C6H3, 215-18°; 6-MeO, 5,2-Cl(MeO)C6H3, 208-11°; 5,6-(MeO)2, PhCH2, 210.2-11.8°; 5,6-EtO(MeO), Ph, 215-22°; 5,6-(MeO)2, 2-pyridyl, 249.6-51.6°; 5,6-(OCH2CH2O), Ph, 172.5-8.5°; 5,6-(MeO)2, 2-EtOC6H4, 135-43°; 5,6-(MeO)2, 2,6-Me2C6H3, 253.2-6.2°; 5,6-(CH2O2), 4-MeOC6H4, 257-8°; 5,6-(CH2O2), 2-BuOC6H4, 164-7.5°; 5,6-(EtO)2, 2-MeOC6H4, 185-6.5°; 5,6-(EtO)2, 3-MeOC6H4, 162-5.5°; H, Ph, 224.2-5.6°; H, PhCH2, 174.4-5.6°; 5,6-(MeO)2, 2-ClC6H4, .apprx.214°; 6-Cl, Ph, 270-4°; 6-MeO, 2-pyridyl, 231-3°; 5,6-(MEO)2, 2-BuOC6H4, 171-4°; 5,6-(MeO)2, 2-EtC6H4, 193-8°; 5,6-(MeO)2, 2,5-(MeO)2C6H3, 208-10°; 5,6-(CH2O2), 2-pyridyl, 271-3°; 5,6-(MeO)2, 2-MeSC6H4, 219-21°. Also prepd. were these III (R1, R2, R3, R4, and m.p. given): H, Ph, Me, H, --; 5,6-(MeO)2, Ph, Me, H, 163-74°; 5,6-(CH2O2), 4-MeOC6H4, Me, H, 173-266°; 5,6-(CH2O2), Ph, H, Me, 219-19.8°; 5,6-(MeO)2, Ph, H, Me, 215-22°; H, Ph, Me, Me, --; 6-MeO, Ph, Me, H, 218-20°; 6-MeO, Ph, Ph, H, 155-60°; 5,6-(MeO)2, 2-MeOC6H4, Me, H, 211.4-12.6°; 5,6-(MeO)2, o-tolyl, Me, H, 119-22°; 5,6-(MeO)2, m-tolyl, Me, H, 120-2°; 5,6-(MeO)2, 3-MeOC6H4, Me, H, 159-63.5°; 5,6-(CH2O2), 2-MeOC6H4, Me, H. 233-5°; 5,6-(MeO)2, Ph, Et, H, 177-84°; 5,6-(EtO)2, Ph, Me, H, 182-7°. A soln. of 41.5 g. X in 250 ml. VIII was added to a suspension of 27 g. LiAlH4 in 300 ml. VIII, and the mixt. refluxed 61/2 hrs. to give 28.5 g. I (R1, R3, R4 = H, R2 = o-tolyl n = 2), m. 124.2-6.4°. Similarly prepd. were these I (R3 = R4 = H, n = 2; R1, R2, and m.p. given): H, H, 149.8-52.0°; H, Me, -- (di-HCl salt m. 279.0-83.8°); H, HOCH2CH2, -- (di-HCl salt m. 266.8-71.4°); H, m-tolyl, 163.8-6.2°; H, 2-MeOC6H4, 111.4-14.2°; H, 4-MeOC6H4, 129.8-31.6°; H, 3,4-ClMeC6H3, 159.2-60.6°; 6-MeO, Ph, 137.4-9.6°; 6-MeO, o-tolyl, 139.2-41.4°; 6-MeO, m-tolyl, 119.8-23.4°; 6-MeO, p-tolyl, 172.2-3.4°; 6-MeO, 2-MeOC6H4, 98.2-100.2°; 6-MeO, 4-MeOC6H4, 185.6-8.6°; 5-PhCH2O, p-tolyl, 151.4-3.6°; 5-PhCH2O, PhCH2CH2, 121-3°; 5-MeS, Ph, 110.2-11.6°; 5-MeS, p-tolyl, 111-13.6°; 5,6-(CH2O2), Ph, 141.0-3.2°; 5,6-(CH2O2), o-tolyl, 159.2-60.8°; 5,6-(CH2O2), m-tolyl, 130.0-1.4°; 5,6-(CH2O2), p-tolyl, 187.0-8.8°; 5,6-(CH2O2), 2-MeOC6H4, 158.0-9.4°; 5,6-(MeO)2, Ph, 128.4-30.0°; 5,6-(MeO)2, o-tolyl, -- (HCl salt m. 218.4-23.4°); 5,6-(MeO)2, m-tolyl, 118.4-19.6°; 5,6-(MeO)2, p-tolyl, 137.8-9.2°; 5,6-(MeO)2,

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2-MeOC6H4, 116.0-16.6°; 5,6-(MeO)2, 3-MeOC6H4, 123.0-4.0°; 5,6-(MeO)2, 4-MeOC6H4, 158.8-64.0°; 5,6-(MeO)2, 4-MeSC6H4, 175.4-7.2°; 5,6-(EtO)2, Ph, 123.0-5.2°; H, 2-pyridyl, -- (HCl salt,m. 232.2-4.4°); 4-MeO, Ph, 177.2-82.2°; 5-MeO, Ph, 147.4-50.0°; 7-MeO, Ph, 122.0-5.2°; 6-Me, Ph, 174.2-5.2°; 6-EtO, Ph, 159.6-63.2°; 6-MeO, 2-ClC6H4, 125.2-8.8°; 6-MeO, 3-ClC6H4, 103.6-4.4°; 6-MeO, 3-MeOC6H4, 142.0-4.6°; 6-MeO, 2-EtOC6H4, 159.4-61.4°; 6-MeO, 2,6-Me2C6H3, 135.2-6.8°; 6-MeO, 2,5-MeOClC6H3, 121.8-8.6°; 5,6-(MeO)2, PhCH2 (XI), 113-14.4°; 5,6-EtO(MeO), Ph, 129.2-30.6°; 5,6-(MeO)2, 2-pyridyl -- (HCl salt m. 210.2-11.8°; 5,6-(OCH2CH2O), Ph, 170.8-6.8°; 5,6-(MeO)2, 2-EtOC6H4, 120.4-2.0°; 5,6-(MeO)2, 2,6-Me2C6H3, 117.8-19.6°; 5,6-(CH2O2), 4-MeOC6H4, 182.4-4.6°; 5,6-(CH2O2), 2-BuOC6H4, 125.0-6.4°; 5,6-(EtO)2, 2-MeOC6H4, 89.4-92.0°; 5,6-(EtO)2, 3-MeOC6H4, 97.6-8.4°; 6-Cl, Ph, 177.2-8.6°; 6-MeO, 2-pyridyl, 107.2-8.2°; 5,6-(MeO)2, 2-BuOC6H4, 93.8-5.8°; 5,6-(MeO)2, 2-EtC6H4, 104.2-7.2°; 5,6-(MeO)2, 2,5-(MeO)2C6H3, 136.8-7.8°; 5,6-(CH2O2), 2-pyridyl, -- (di-HCl salt m. 200-24°); 5,6-(MeO)2, 2-MeSC6H4, 116-17.8°. Also made were these I (n = 2; R1, R2, R3, R4, and m.p. given): H, Ph, Me, H, 154.2-5.6°; 5,6-(MeO)2, Ph, Me, H, -- (HCl salt m. 249.0-55.4°); 5,6-(CH2O2), 4-MeOC6H4, Me, H, 160.8-2.8°; 6-MeO, Ph, Me, H, -- (HCl salt m. 253.2-6.2°); 6-MeO, Ph, Ph, H, 148.2-8.8°; 5,6-(MeO)2, 2-MeOC6H4, Me, H, -- (di-HCl salt m. 217.4-20.8°); 5,6-(MeO)2, o-tolyl, Me, H, 119.8°-21.6°; 5,6-(MeO)2, m-tolyl, Me, H, -- (di-HCl salt m. 210.2-3.8°); 5,6-(MeO)2, 3-MeOC6H4, Me, H, -- (di-HCl salt m. 182.6-4.2°); 5,6-(CH2O2), 2-MeOC6H4, Me, H, 137.0-43.0°; 5,6-(CH2O2), 2-MeOC6H4, H, Me, 155.4-6.4°; 5,6-(MeO)2, Ph, Me, H, 139.6-40.4°; 5,6-(MeO)2, Ph, Et, H, --(HCl salt m. 237.6-9.0°); 5,6-(EtO)2, Ph, Me, H, 111.6-13.2°; 5,6-(CH2O2), 2-MeOC6H4, Me, Me, 118.2-19.6°; 5,6-(CH2O2), 2-MeOC6H4, Me, PhCH2, 169.2-70.2°; H, 2-MeOC6H4, H, Me, 74.6-6.4°. Catalytic debenzylation of XI gave I (R1 = 5,6-(MeO)2, R2, R3, R4 = H, n = 2), m. 109.6-11.4°, which reacted with 2-chloropyrimidine to give I (R1 = 5,6-(MeO)2, R2 = 2-pyrimidinyl, R3, R4 = H, n = 2), m. 127.2-8.2°. III (R4 = alkyl was reduced to II; other II were obtained as by-products in the LiAlH4 redn. of III. Thus were made these II (n = 1; R1, R2, R3, R4, and m.p. given): 5,6-(CH2O2), Ph, H, Me, 171-2.5°; 5,6-(MeO)2, Ph, H, Me, 128.4-30.2°; H, Ph, Me, Me, 136.8-9.6°; 5,6-(MeO)2, p-tolyl, H, H, 193.2-8.0°. Method C: On addn. of 3-(4-benzhydryl-1-piperazinyl)propionyl chloride to a soln. of 5-chloroindole and EtMgBr in ether, there was obtained IV (R1 = 5-Cl, R2 = Ph2CH, R3, R4 = H, n = 2) (XII), which with MeI and NaNH2 in liquid NH3 gave IV (R1 = 5-Cl, R2 = Ph2CH, R3 = H, R4 = Me, n = 2). Similarly made were these IV (R1, R2, R3,R4, and n given): H, Ph, Ph, H, 3; H, Ph, Ph, PhCH2, 3. XII was reduced by LiAlH4 to I (R1 = 5-Cl, R2 = Ph2CH, R3, R4 = H, n = 3), but XII reduced by NaBH4 yielded II (R1 = 5-Cl, R2= Ph2CH, R3 = R4 = H, n = 2). When IV (R4 = alkyl) was reduced by LiAlH4, then II was obtained. Thus were made these II (R1, R2, R3, R4 and n given): 5-Cl, Ph2CH, H, Me, 2; H, Ph, Ph, PhCH2, 3; 6-BuO, Me, H, 4-MeSC6H4CH2CH2, 3; 5,6,7-(MeO)3, Me, H,

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4-BuOC6H4CH2CH2, 3; H, Me, H, 3-HOC6H4CH2CH2, 3; H, Me, H, PhCH:CHCH2, 3. Method D: To a cold soln. of 22.5 g. 3-indoleacetic acid and 13.3 g. Et3N in 800 ml. Me2CO was added 18.1 g. ClCO2Bu-iso, the mixt. stirred for 10 min. at -10°, a soln. of 1-phenylpiperazine in little Me2CO added, and the mixt. kept 1.7 hrs. at room temp. to yield 5.4 g. V(R1, R2 = H, R3 = Ph, n = 1), m. 179.4-81.6°. Similarly prepd. were these V (R3 = H; R1, R2, n, and m.p. given): H, Ph, 2, 136.2-7.4°; H, 3-MeOC6H4, 1, --; H, 2-ClC6H4, 2, --; H, o-tolyl, 2, --; H, 2-MeOC6H4, 2, 173.0-6.0°; H, Ph, 3, --; H, 2-MeOC6H4, 3, 129-32°; H, 3-MeOC6H4, 3, --; 6-MeO, Ph, 2, 169-72°; 6-MeO, 2-MeOC6H4, 2, 120.5-2.0°; 5,6-(MeO)2, 3-ClC6H4, 1, --; 5,6-(CH2O2), Ph, 2, 178-80°; 5,6-(MeO)2, 2-ClC6H4, 1, 185-8.5°; 5,6-(MeO)2, 2-MeOC6H4, 2, 124.8-7.4°; 5,6-(MeO)2, Ph, 2, 120.5-2.0°; 5,6-(MeO)2, 3-MeOC6H4, 2, --. Also obtained was V [R1 = 5,6-(MeO)2, R2 = Ph, R3 = Me, n = 2). Also made was 1-[3-(1-indolyl)propionyl]-4-phenylpiperazine, an oil and 1-[3-(2-methyl-5,6-dimethoxy-3-indolyl)propionyl]-4-phenylpiperazine. By redn. of these V by LiAlH4 in VIII were prepd. these I (R3 = R4 = H; R1, R2, n, and m.p. given): H, Ph, 2, --; H, Ph, 3, 126.6-7.8°; H, 3-MeOC6H4, 2, 146.4-7.6°; H, 2-ClC6H4, 3, 140.3-3.6°; H, o-tolyl, 3, 102.4-4.2°; H, 2-MeOC6H4, 3, 156.8-9.2°; H, Ph, 4, 96.0-100.8°; H, 2-MeOC6H4, 4, 120.6-3.8°; H, 3-MeOC6H4, 4, -- (HCl salt, m. 234.2-5.8°); 6-MeO, Ph, 3, 196.4-7.6°; 6-MeO, 2-MeOC6H4, 3, 153.2-5.0°; 5,6-di-MeO, 3-ClC6H4, 2, --(HCl salt m. 236.8-9.2°); 5,6-(CH2O2), Ph, 3, 142.6-4.2°; 5,6-(MeO)2, 2-ClC6H4, 2, 86.8-9.8°; 5,6-(MeO)2, 2-MeOC6H4, 3, 120.4-1.4°; 5,6-(MeO)2, Ph, 3, 157.4-8.2°; 5,6-(MeO)2, 3-MeOC6H4, 3, 159.0-60.2°. Also made was I (R1 = 5,6-(MeO)2, R2= Ph, R3 = Me, R4 = H, n = 3), m. 117.8-18.8°, and 1-[3-(1-indolyl)propyl]-4-phenylpiperazine, m. 96.7-8.4°. Method E: A soln. of 9.0 g. indole in 100 ml. dioxane was added to a cold soln. of 6.25 ml. 40% aq. CH2O and 13.3 g. 1-phenylpiperazine in 1 l. dioxane to give I (R1 = R3 = R4 = H, R2 = Ph, n = 1), m. 184.6-6.8°. Similarly made was I (R1 = 5,6-(MeO)2, R2 = Ph, R3 = R4 = H, n = 1), m. 159.3-60.2°. Method F: The piperazine ring was formed after a substituted ethylenediamine group had been joined to the indole moiety. Thus, 27 g. IX and 58 g. (PhCH2)NPhCH2CH2NH2 in 300 ml. VIII refluxed for 5 hrs. gave 41.9 g. N-benzyl-N-phenyl-N'-[(3-indolyl)glyoxalyl]ethylenediamine, m. 162.2-2.8°, which was reduced by LiAlH4 to N-benzyl-N-phenyl-N'-[2-(3-indolyl)ethyl]ethylenediamine (XIII) (di-HCl salt m. 171.4-5.4°). Also made were N-benzyl-N-methyl-N'-[(3-indolyl)glyoxalyl]ethylenediamine, m. 124.5-7.0°, and N-benzyl-N-methyl-N'-[2-(3-indolyl)ethyl]ethylenediamine, m. 102-5°. A soln. of 11.1 g. XIII and 3.4 g. ClCH2COCl in CH2Cl2 was refluxed to yield 9.4 g. 4-[2-(3-indolyl)ethyl]-1-phenyl-1-benzyl-1m3-oxopiperazinium chloride, m. 157-9.5°, which was catalytically debenzylated to 1-[2-(3-indolyl)ethyl]-4-phenyl-2-piperazinone, m. 157.2-9.0°. Similarly made was 4-[2-(3-indolyl)ethyl]-1-methyl-1-benzyl-3-oxopiperazinium chloride, m. 229.5-32.5°, and 4-[2-(3-indolyl)ethyl]-2-methyl-1-phenyl-3-piperazinone, m. 186.4-91.8°. The latter, reduced by LiAlH4, gave 1-[2-(3-indolyl)ethyl]-3-methyl-4-phenylpiperazine, m. 116.2-17.6°.

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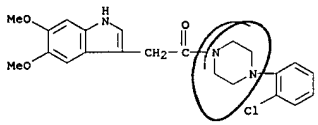
IT 96266-49-8P, Piperazine, 1-(o-chlorophenyl)-4-[(5,6-dimethoxyindol-3-yl)acetyl]-
RL: PREP (Preparation)
(preparation of)
RN 96266-49-8 CAPLUS
CN Piperazine, 1-(o-chlorophenyl)-4-[(5,6-dimethoxyindol-3-yl)acetyl]- (7CI) (CA INDEX NAME)



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ACCESSION NUMBER: 1962:449171 CAPLUS
DOCUMENT NUMBER: 57:49171
ORIGINAL REFERENCE NO.: 57:9785b-i,9786a-i,9787a-b
TITLE: Research in the indole series. VI. Some substituted tryptamines
AUTHOR(S): Julia, Marc; Igolen, Jean; Igolen, Hanne
SOURCE: Bulletin de la Societe Chimique de France (1962) 1060-8
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB A series of substituted 3-indolylacetic acids was prepared from secondary aromatic amines and 4-bromo-3-oxo esters; the acids were converted via the amides or the alcs. and bromides to the corresponding tryptamines. PhNH2 (279 g.) and 185 g. PhCH2CH2Br (I) in 500 cc. dry xylene refluxed 12 h. gave 151 g. PhNHCH2CH2Ph, b0.4 155-60°. p-MeOC6H4NH2 (295 g.) and 148 g. I in 350 cc. xylene gave similarly 95 g. unreacted p-MeOC6H4NH2 and 135 g. yellow-green oily p-MeOC6H4NHCH2CH2Ph (II), b0.1 170-5°; HCl salt m. 127-8° (EtOH-Et2O). p-MeOC6H4NH2 (3 mol) and Ph(CH2)3Br gave p-MeOC6H4NH(CH2)3Ph, b0.2 180-90°, needles, m. 44° (EtOH); HCl salt, plates, m. 158-9° (H2O); HBr salt, needles, 129° (EtOH). 4-Aminoveratrole gave similarly 89% 3,4-(MeO)2C6H3NHCH2Ph, b0.2 170-2° [HCl salt, plates, m. 142-5° (iso-PrOH)], and 3,4-(MeO)2C6H3NHC6H4OMe-p, 72%, needles, 86.5° (EtOH); HCl salt m. 188° (EtOH). By the direct bromination of the corresponding oxoesters were prepared the following compds.: MeCHBrCOCH2CO2Et, 73%, b0.25 82-5°; BrCH2COCHMeCO2Et, 65%, b0.2 80-5°; BrCH2COCMe2CO2Et, 95%, -(crude); BrCH2COCH(OCEt)CO2Et, 66, b0.1 69-72°. II (209 g.) and 96.1 g. BrCH2COCH2CO2Et (III) diluted with cooling with 250 cc. dry Et2O, filtered from 138 g. II.HBr, evaporated, the residue refluxed 15 h. with 63 g. ZnCl2 in 250 cc. absolute EtOH, evaporated, treated with H2O and C6H6, and the organic layer worked up gave 113 g. Et ester (IV) of 1-phenethyl-5-methoxy-3-indolylacetic acid (V), b0.1 215-20°, yellow-orange oil, which refluxed 1-2 h. with KOHMeOH yielded 73% V, m. 129-31° (aqueous EtOH); method A. III (50 g.) and 100 g. p-MeOC6H4NHCH2Ph in 300 cc. absolute EtOH refluxed 40 h., evaporated, the residue treated with H2O and Et2O, and the Et2O phase worked up yielded 44.7 g. Et ester (VI) of 1-benzyl-5-methoxy-3-indolylacetic acid (VII), b0.15 180-5°, yellow-orange oil, which saponified in the usual manner yielded 84% VII, m. 128-9°; method B. VI was also obtained in 64% yield by method A. In the same manner were prepared the following VIII (X, R1, R2, R3, R4, method, % yield of Et ester, b.p./mm. or m.p. of Et ester, % yield of free VIII, m.p., and m.p. of corresponding skatole given): H, PhCH2CH2, H, H, H, A, 68, 204-8°/0.15, 90, 103° (C6H6) (IX), -; 5-MeO, p-MeOC6H4CH2, H, H, H, A, 55 (47% by method B), 220-8°/0.05 [m. 50-2° (EtOH)], 85, 116-18° (EtOH) (X), -; 5-MeO, Ph(CH2)3, H, H, H, A, 72, 230-5°/0.4 (XI), 50, 86° (Et2O-petr. ether) (XII), -; 5,6-(MeO)2, PhCH2, H, H, H, A, 69, 215-25°/0.15 (m. 64-5°), 82, 141° (EtOH) (XIII), 81.5°; 5,6-(MeO)2, p-MeO-C6H4CH2, H, H, H, B, 82, 86-5.8° (EtOH), 100, 127° (EtOH) (XIV), 102° (EtOH); 5-MeO, PhCH2,

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Me, H, H, A, 48, 201-5°/0.01 (m. 70.5-1.5°), 82,
173-4° (EtOH) (XV), --; 5-MeO, PhCH2, H, Me, H, A, 20,
200-10°/0.6, 45, 108° (Et2O-petr. ether) (XVI), --; 5-MeO,
PhCH2, H, Me, Me, A, 65, 210-30°/0.25 (m. 80°), 70,
151-2° (EtOH) (XVII), 58° (EtOH); H, PhCH2, Me, Me, H, A, 26
(43% by method B), 178-81°/0.05, 63, 160-2° (aq. EtOH)
(XVIII), --; 5-MeO, PhCH2, Me, Me, H, A, 41 (30% by method B),
190-3°/0.1 [m. 80-1° (MeOH)], 89, 148-51° (EtOH), --;
5-MeO, p-MeOC6H4CH2, Me, Me, H, A, 28, 208-12°/0.1, 76,
159-60° (EtOH), --. IV (8 g.) in 80 cc. MeOH (satd. with NH3)
heated 24 h. in a sealed tube at 105°, filtered, and evapd. gave
5.2 g. 1-phenethyl-5-methoxy-3-indolylacetamide (XIX), needles, m.
147-8° (abs. EtOH); method D. The amides were also prepd. by
heating the acid with urea; method C. XI (13.6 g.) in 200 cc. CHCl3 and
4.26 g. Et3N cooled to -5°, treated rapidly with 4.58 g. ClCO2Et,
stirred 15 min., treated 5 min. with a stream of dry NH3, kept 1 h. at
room temp., dild. with H2O, and the CHCl3 layer worked up gave 7.7 g.
amide of XII, needles, m. 124-5°; method E. Similarly were prepd.
the amides of the following compds. (m.p., % yield, and method given):
IX,
146-7° (C6H6), 70, C; VII, 156-7°, 70, C (69% by method E);
X, 138.5-9.5° (EtOH), 81, C (66% by method D); V, 147-8°
(EtOH), 74, D; XII, 1245° (C6H6-petr. ether), 57, E; XIII,
167-8° (EtOH), 67, D; XIV, 166° (EtOH), 95, D; XV,
129-30° (EtOAc-petr. ether), 70, C; XVI, 180.5-82° (EtOH),
39, C; XVII, 183° (EtOH), 81, E; XVIII, 163-4° (EtOH), 70,
C. By the same methods were prepd. the dimethylamides of the following
acids (same data given): IX, -- (oil), 80, E [picrate m. 84°
(EtOAc-petr. ether)]; V, --, 94, E; XII, --, 75, E [picrate m. 97°
(EtOAc-petr. ether)]. The diethylamides of the following acids (same
data
given): IX, 63-4° (Et2O), 50, E [picrate m. 104-5°
(EtOH-Et2O)]; V,--, 85, E [picrate m. 103-4° (EtOH-Et2O)]; XII, --,
75, E [picrate m. 117° (EtOAc-petr. ether)]. X (0.5 g.) and 0.17
g. PhNH2 in 5 cc. CH2Cl2 treated with 0.33 g. dicyclohexyldicarbodiimide,
kept 16 h. at room temp., filtered from 0.26 g. dicyclohexylurea, treated
with AcOH to ppt. an addnl. 0.08 g. urea, and the filtrate worked up gave
0.4 g. anilide of X, m. 133° (aq. EtOH). VI (28 g.) in 100 cc.
Et2O added gradually at 0° to 4 g. LiAlH4 in 900 cc. Et2O, refluxed
3 h., and worked up gave 21 g.
1-benzyl-3-(2-hydroxyethyl)-5-methoxyindole
(XX), b0.05 172-8°, m. 47-8° (Et2O-petr. ether);
3,5-dinitrobenzoate, red crystals, m. 158-61° (EtOAc). Similarly
were prepd. the 3-(2-HOCH2CH2) analogs of the following compds. (b.p./mm.
and % yield given): X, 185-95°/0.05, 79 [3,5-dinitrobenzoate m.
169-71° (EtOH-Et2O)]; XIII, 95-6° (Et2O-petr. ether), 91; V,
195°/0.1, 78 [picrate m. 79-81° (C6H6-petr. ether)]; XVIII,
89°, 65; XIV, 81-2° (Et2O), 80. XX (3 g.) in 140 cc. dry
Et2O treated dropwise at 0° with 1.8 g. PBr3 in 30 cc. Et2O, kept
16 h. at room temp., decanted, the residual resin extd. with Et2O, and
the
ext. worked up gave 2.5 g. 1-benzyl-3(2-bromoethyl)-5-methoxyindole,
prisms, m. 94-5° (abs. EtOH). Similarly were prepd. the
3-(2-BrCH2CH2) analogs of the following compds. (m.p. and % yield given):
V, --, 45; XIII, 77-8° (EtOH), 55; XVIII, 89°, 65. XIX (5.5

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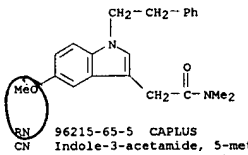
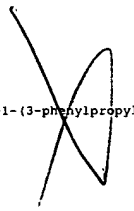
g.) and 1.4 g. LiAlH4 in 500 cc. Et2O refluxed 66 h. and worked up in the
usual manner yielded 1-phenethyl-5-methoxy-3-(2-aminoethyl)indole-HCl, m.
136-8° (abs. EtOH). Similarly were prepd. the 3-(2-H2NCH2CH2)
analog HCl salts of the following compds. (m.p. and % yield given): IX
(XXI), 128-30° (EtOAc), 72; VII, 156-9° (EtOH-Et2O), 74
[picrate m. 167-8° (EtOH)]; X, 162-4° (EtOH-Et2O), 71; V,
136-8° (EtOH), 74; XII, 124-6° (EtOH-Et2O), 70; XIII,
95-6° (Et2O-petr. ether), 91; XIV, -- (hygroscopic), 42 [picrate m.
190-3° (EtOH)]; XV (XXII), 229-31° (EtOH), 52; XVI,
168-73° (EtOH-Et2O), 68; XVII, 228-32° (EtOH-Et2O), 73;
XVIII, 78-80° (iso-PrOH), 50. The 3-(2-Me2NCH2CH2) analog HCl
salts of the following compds. (same data given): IX (XXIII),
199-200° (EtOH), 58; VII, 189-91° (EtOH), 50; X,
174-6° (EtOH), 55; V (XXIIIA), 122-4° (iso-PrOH-Et2O), 60
(44) [methiodide m. 194-6° (EtOH), 75%]; XII, 143-5°
(EtOH-Et2O), 66; XIII, -- (hygroscopic), 35 [picrate m. 172-4°
(EtOAc)]; XVIII, 193-4° (EtOH), 86. In the same manner were prepd.
the 3-(Et2NCH2CH2) analog HCl salts of the following compds. (same data
given): IX (XXIV), 104-5° (EtOH-Et2O), 72; X, --, 65 [picrate m.
88-9° (C6H6)]; V (XXV), 99-100° (EtOH-Et2O), 60; XII, --
(hygroscopic), 45; XVIII, 167-9° (EtOH-iso-Pr2O), 30.
1-Benzyl-5-methoxy-3-(2-piperidinoethyl)indole-HCl, m. 202-4°
(iso-PrOH), was obtained in 60% yield by heating the corresponding
3-(2-BrCH2CH2) analog (2 g.) with 1.5 g. piperidine in 65 cc. MeOH 15 h.
in a sealed tube at 100°. Similarly was prepd. the
3-(2-piperidinoethyl) analog HCl salt of X, m. 180-3° (iso-PrOH),
in 56% yield. VI (1.62 g.) and 0.32 g. N2H4.H2O in 20 cc. abs. EtOH
refluxed 20 h., cooled, and filtered yielded 1.1 g. hydrazide of VII, m.
140° (EtOH). Similarly were prepd. the hydrazides of the following
acids (m.p. and % yield given): IX, 128-30° (EtOH), 50; X,
144-6° (EtOH), 61; V, 117-18° (EtOH), 68; XIII,
173.5° (EtOH), 63; XIV, 179-82° (EtOH), 82. VII (5.1 g.)
and 3.1 g. NaOAc in 10 cc. Ac2O refluxed 18 h., cooled, worked up, and
the
crude product (1.85 g.) chromatographed on Al2O3 gave 409 mg.
1-benzyl-5-methoxy-3-acetonylindole, m. 62.5-3.5° (Et2O-petr.
ether); 2,4-dinitrophenylhydrazone, orange prisms, m. 62.5-63°
(EtOAc); oxime (XXVI), prisms, m. 98.5-9.5° (C6H6-petr. ether).
Similarly was prepd. the 3-acetonyl analog of XIII in 56% yield;
2,4-dinitrophenylhydrazone m. 186° (EtOH). In the same manner as
XXI was prepd. the 3-(2-H2NCHMeCH2) analog HCl salt of VII, 71%, m.
190-2° (EtOH-Et2O), and the 3-(PhCH2NMeCH2CH2) analog HCl salt of
X, 32%, m. 160° (EtOH-Et2O). The antiserotonin activities of XXI,
XXIII, XXIIIA, XXIV, and XXV were detd. XXII did not show any
tuberculostatic activity in vivo at the max. tolerable dose.
IT 94916-80-0P, Indole-3-acetamide, 5-methoxy-N,N-dimethyl-1-
phenethyl- 96215-65-5P, Indole-3-acetamide, 5-methoxy-N,N-
dimethyl-1-(3-phenylpropyl)-, picrate 96310-29-1P,
Indole-3-acetamide, N,N-diethyl-5-methoxy-1-phenethyl-, picrate
97076-37-4P, Indole-3-acetamide, N,N-diethyl-5-methoxy-1-(3-
phenylpropyl)-, picrate
RL: PREP (Preparation)
(preparation of)
RN 94916-80-0 CAPLUS
CN Indole-3-acetamide, 5-methoxy-N,N-dimethyl-1-phenethyl- (7CI) (CA INDEX

L3 ANSWER 64 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
NAME)

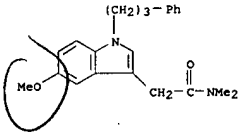




RN 96215-65-5 CAPLUS
CN Indole-3-acetamide, 5-methoxy-N,N-dimethyl-1-(3-phenylpropyl)-, picrate
(7CI) (CA INDEX NAME)

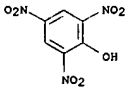
CM 1

CRN 96215-64-4
CMF C22 H26 N2 O2



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7

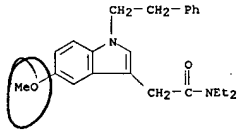


RN 96310-29-1 CAPLUS
CN Indole-3-acetamide, N,N-diethyl-5-methoxy-1-phenethyl-, picrate (7CI)
(CA
INDEX NAME)

CM 1

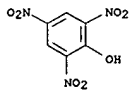
CRN 96310-28-0
CMF C23 H28 N2 O2

L3 ANSWER 64 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



CM 2

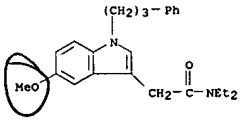
CRN 88-89-1
CMF C6 H3 N3 O7



RN 97076-37-4 CAPLUS
CN Indole-3-acetamide, N,N-diethyl-5-methoxy-1-(3-phenylpropyl)-, picrate
(7CI) (CA INDEX NAME)

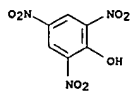
CM 1

CRN 97076-36-3
CMF C24 H30 N2 O2



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



L3 ANSWER 64 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)

L3 ANSWER 65 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1962:449170 CAPLUS
DOCUMENT NUMBER: 57:49170
ORIGINAL REFERENCE NO.: 57:9784b-i,9785a-b
TITLE: Research in the indole series. V. Preparation of 3-indolylacetamides and tryptamines
AUTHOR(S): Julia, Marc; Igolen, Jean
SOURCE: Bulletin de la Societe Chimique de France (1962) 1056-60
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 57:49170
AB A series of 3-indolylacetamides was prepared from 4-bromoacetoacetamides with secondary aromatic amines and reduced to the corresponding tryptamines, p-MeOC6H4CH:NPh in AcOEt hydrogenated over PtO2 yielded p-MeOC6H4CH2NHPh (I), b15 206-8°, m. 48-9°. p-MeOC6H4CH:NC6H4OMe-p, m. 142° (EtOH), in EtOAc hydrogenated over Raney Ni at 75°/150 atmospheric yielded 90% p-MeOC6H4CH2NHC6H4OMe-p (II), plates, m. 94-5° (EtOH). 3,4-(EtO)2C6H3CH:NC6H4OMe-p, m. 96-8° (EtOH), in EtOAc hydrogenated under ambient conditions over PtO2 yielded 80% 3,4-(EtO)2C6H3CH2NHC6H4OMe-p (III), b0.15 210-12°, m. 54-5° (petr. ether). N-Piperonylidene-p-anisidine, m. 119-20° (EtOH), gave similarly N-piperonyl-p-anisidine (IV), m. 76-8° (EtOH). AcCH2CONEt2 (15.7 g.) treated with 16.0 g. Br in 90 cc. CHCl3 gave 20 g. crude BrCH2COCH2CONEt2 (V), yellow oil, which decomposed rapidly at 100° and was used without purification. BrCH2COCH2CONHPh (VI) (5.12 g.) in 12 cc. HCONMe2 and 4.28 g. MeNHPh in 6 cc. HCONMe2 kept overnight, diluted with 300 cc. H2O, extracted with C6H6, the aqueous layer basified, and extracted with Et2O gave 1.42 g. MeNHPh; the C6H6 phase worked up yielded 4.15 g. p-MeC6H4NHCH2COCH2CONHPh (VII), m. 90-1° (80% EtOH). VII (4 g.) and 4 g. ZnCl2 heated 45 min. at 100-10°, cooled, dissolved with heating in 40 cc. 4N HCl, extracted with C6H6, and the extract worked up gave 3.4 g. crystals, m. 92-112°, which chromatographed from C6H6 on Al2O3 yielded 2.65 g. 1-methyl-3-indolylacetamide (VIII), needles, m. 111-12° (80% EtOH); method A. VI (5.12 g.), 4.28 g. MeNHPh, and 90 cc. absolute EtOH refluxed 18 hrs., concentrated, diluted with 200 cc. H2O, extracted with C6H6, and the aqueous phase worked up yielded 1.75 g. MeNHPh; the C6H6 extract yielded 1.8 g. (crude) VIII, m. 111-12°; method B. VIII (200 mg.) and 15 cc. 5N HCl refluxed 1.5 hrs., refrigerated overnight, and filtered gave 1-methyl-3-indolylacetic acid, m. 125-7° (H2O). Similarly were prepared the following compds. (appearance, m.p., acetoacetanilide, secondary amine, and % yields by methods A and B obtained given): 1-ethyl-3-indolylacetanilide (IX), prisms, 104-5° (70% EtOH), VI, EtNHPh, 3.1, 2.1; 1-benzyl-3-indolylacetanilide (X), needles, 127-8° (EtOH), VI, PhNHCH2Ph, 2.4, 1.5; 5-MeO derivative of X, --, 136-7° (70% EtOH), VI, p-MeOC6H4NHCH2Ph (XI), 1.1, 1.4; 5-PhCH2O derivative (XII) of VIII, --, 162-4° (C6H6), VI, p-PhCH2OC6H4NMePh, --, 4.5; 1-anisyl-3-indolylacetanilide (XIII), needles, 130-1° (absolute EtOH), VI, I, --, 2.3; 5-MeO derivative (XIV) of XIII, prisms, 134° (80% EtOH), VI, II, 5.2, 4.8; 1-(3,4-diethoxybenzyl)-5-methoxy-3-

L3 ANSWER 65 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
indolylacet anilide (XV), needles, 134-6° (MeOH), VI, III, --, 4.1; 1-piperonyl analog (XVI) of XV, needles, 158-9° (C6H6), VI, IV, --, 5.5; N,N-di-Et deriv. (XVII) of VIII, --, 80-1° (petr. ether), V, MeNHPh, 0.25, -- [picrate m. 124-6° (C6H6-petr. ether)]; N,N-di-Et deriv. (XVIII) of IX, yellow oil, --, V, EtNHPh, 6.7, -- [picrate, yellow-orange needles, m. 109-11° (C6H6-petr. ether)]; N,N-di-Et deriv. of X, prisms, 95-6° (60% EtOH), V, PhNHCH2Ph, 5.3, -- [PhCH2NPhCH2COCH2NEt2, 7.1 g., needles, m. 103-5° (abs. EtOH), was obtained as the intermediate]; 1-benzyl-5-methoxy-3-indolyl(N,N-diethyl)acetamide (XIX), -- (oil), --, V, XI, 12.1, -- [picrate, yellow needles, m. 133-5° (C6H6-petr. ether)]. X (1 g.), 0.25 g. LiAlH4, and 300 cc. Et2O refluxed 14 hrs., worked up, and the base isolated as the HCl salt gave 400 mg. 1-benzyl-3-(2-phenylaminoethyl)indole-HCl (XX), m. 136-8° (C6H6-petr. ether). XII (2.2 g.), 0.6, LiAlH4, and 1100 cc. Et2O refluxed 18 hrs. gave similarly 1.1 g. 5-PhCH2O deriv. of XX, m. 151-4° (isoPrOH). Powd. XIV (5 g.), 3 g. LiAlH4, and 1600 cc. dry Et2O refluxed 27 hrs., worked up, the yellow oily residue dissolved in Et2O, and treated with dry HCl gave 3.8 g. 1-anisyl-5-methoxy-3-(2-anilinoethyl)indole-HCl, m. 147-9° (abs. EtOH). Similarly were prepd. the following compds. (m.p. given): 1-anisyl-3-(2-anilinoethyl)indole-HCl, 151-3° (abs. EtOH)(needles); 1-piperonyl-5-methoxy-3-(2-anilinoethyl)indole-HCl (XXI), 172-5° (abs. EtOH) (needles); 1-[3,4-(EtO)2C6H3CH2] analog of XXI, 142-4° (iso-PrOH); 1-methyl-3-(2-diethylaminoethyl)indole-HCl (XXII), 203° (abs. EtOH) (needles); 1-Et homolog of XXII, 115-16° (iso-PrOH); 1-benzyl-5-methoxy-3-(2-diethylaminoethyl)indole-HCl, 135° (iso-PrOH).

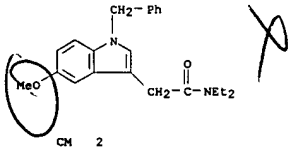
IT 96215-63-3P, Indole-3-acetamide, 1-benzyl-N,N-diethyl-5-methoxy-, picrate
RL: PREP (Preparation)
(preparation of)

RN 96215-63-3 CAPLUS

CN Indole-3-acetamide, 1-benzyl-N,N-diethyl-5-methoxy-, picrate (7CI) (CA INDEX NAME)

CM 1

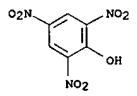
CRN 96215-62-2
CMF C22 H26 N2 O2



CM 2

CRN 88-89-1
CMF C6 H3 N3 O7

L3 ANSWER 65 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)



L3 ANSWER 66 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1956:89506 CAPLUS
DOCUMENT NUMBER: 50:89506
ORIGINAL REFERENCE NO.: 50:16869h-i,16870a-f
TITLE: (5-Benzyloxy-3-indole)alkylamines
PATENT ASSIGNEE(S): Upjohn Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

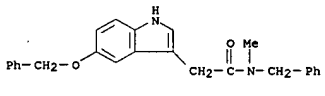
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 744773		19560215	GB 1953-8777	19530330

AB Compds. possessing vasoconstrictor properties are prepared by coupling a Grignard reagent prepared from Me2NCO(CH2)nCHRX (R = alkyl, X = halogen) with a 2-alkyl-5-benzyloxyindole giving a 2-alkyl-5-benzyloxy-3-indolealkanoylamide which is reduced to a 2-alkyl-5-benzyloxy-3-indolealkylamine. Thus to 4.25 g. 4.25 g. MeI and 2.4 g. Mg in 200 ml. Et2O was added 5.5 g. 5-benzyloxyindole in 200 ml. Et2O. After refluxing 30 min., cooling in ice and adding 5.9 g. of BzMeNCOCH2Cl in 500 ml. Et2O, the Et2O was distilled off and the residue heated 3 hrs. on the steam bath, taken up in Et2O, and decomposed with 5% AcOH, giving 7,5 g. N-methyl-N-benzyl-α-(5-benzyloxy-3-indolyl)acetamide (I), m. 151-2° (from iso-PrOH). I reduced with LiAlH4 in tetrahydrofuran gave after acidification with HCl, 71% 5-benzyloxy-3-[2-(N-benzyl-N-methylamino)ethyl]indole hydrochloride, C25H26N2O.HCl, m. 110-12°. Similarly were prepared the following 5-benzyloxy-3-R-substituted indoles (R, m.p., m.p. of hydrochloride, and % yield given): (PhCH2)2NCH2CH2, 101-2°, 232-3°, 65; Me2NCH2CH2, -, 154-5°, 29; 2-piperidinoethyl, -, 208-9.5°, 11.5; Bu2NCH2CH2, -, 218-20°, -; PhCH2(PhCH2CH2)NCH2CH2, -, 214-15°, -. Also prepared without phys. consts. given were 2-ethyl-5-benzyloxy-3-(2-piperidinoethyl)indole, 5-benzyloxy-3-(1-methyl-2-piperidinoethyl)indole, 5-benzyloxy-3-(2-morpholinoethyl)indole, 5-benzyloxy-3-[2-(1-pyrrolidinyl)ethyl]indole, 5-benzyloxy-3-(2-thiamorpholinoethyl)indole, 5-benzyloxy-3-(3-piperidinopropyl)indole, 5-benzyloxy-3-(1-ethyl-3-piperidinopropyl)indole, 5-p-methylbenzyloxy-3-[2-(N-benzylamino)ethyl]indole, 5-(p-propylbenzyloxy)-3-[2-(N-isopropyl-N-benzylamino)ethyl]indole, 2-methyl-5-(p-ethylbenzyloxy)-3-[2-(N-phenylamino)ethyl]indole, 5-(p,p'-dimethylbenzhydryloxy)-3-[2-(N-isopropylamino)ethyl]indole, 5-(p-ethylbenzyloxy)-3-[3-(N-benzylamino)propyl]indole, 5-(p-iodobenzyloxy)-3-[2-(N,N-dicyclohexylamino)ethyl]indole, 5-(p,p'-dichlorobenzhydryloxy)-3-[1-ethyl-2-(N-methyl-N-benzylamino)ethyl]indole, 5-(p,p'-dichlorobenzhydryloxy)-3-[3-(N-isopropylamino)propyl]indole, 5-(p-bromobenzyloxy)-3-[1-ethyl-3-(N-methylamino)propyl]indole, 5-(p-methoxybenzyloxy)-3-[2-(N,N-dicyclohexylamino)ethyl]indole, 5-(p,p'-dimethoxybenzhydryloxy)-3-[1-propyl-2-(N-ethyl-N-cyclohexylamino)ethyl]indole, 2-propyl-5-(p-ethoxybenzyloxy)-3-[2-(N-benzylamino)ethyl]indole, 5-(p,p'-dimethoxybenzhydryloxy)-3-[2-(N,N-dibenzylamino)ethyl]indole, 5-(p-ethoxybenzyloxy)-3-[1-ethyl-3-(N-benzylamino)propyl]indole, 5-benzyloxy-3-[3-(N-isopropylamino)propyl]indole, 5-benzyloxy-3-[3-(N,N-

L3 ANSWER 66 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN (Continued)
dimethylamino)propyl]indole, 5-benzyloxy-3-[3-(N-methyl-N-benzylamino)propylindole, 5-benzyloxy-3-[1-methyl-3-(N-benzylamino)propyl]indole, 2-ethyl-5-benzyloxy-3-[3-(N-benzylamino)propyl]indole, 5-benzhydryloxy-3-[2-(N-cyclopentyl-N-ethylamino)ethylindole, 5-benzhydryloxy-3-[1-ethyl-2-(N,N-diphenylamino)ethyl]indole, 2-methyl-5-benzhydryloxy-3-[2-(N-benzyl-N-methylamino)ethyl]indole, 5-benzhydryloxy-3-[3-(N-methyl-N-benzylamino)propyl]indole, 5-benzhydryloxy-3-[1-ethyl-3-(N-methylamino)propyl]indole, 5-benzyloxy-3-[1-methyl-2-(N-benzylamino)ethyl]indole, 2-methyl-5-benzyloxy-3-[2-(N,N-dicyclohexylamino)ethyl]indole, 5-benzyloxy-3-[2-(N-cyclohexylamino)ethyl]indole, 5-benzyloxy-3-(2-(N-methylamino)ethyl]indole, 5-benzyloxy-3-[3-(N-methyl-N-benzylamino)propyl]indole, and 5-benzyloxy-3-[1-methyl-3-(N-benzylamino)propyl]indole. Cf. Brit. 744,774 (following abstr.) and C.A. 50, 5035h.

IT 725227-53-2P, 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-methyl-
RL: PREP (Preparation)
(preparation of)

RN 725227-53-2 CAPLUS
CN 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-methyl- (5CI) (CA INDEX NAME)



See 69

L3 ANSWER 67 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1956:27880 CAPLUS
DOCUMENT NUMBER: 50:27880
ORIGINAL REFERENCE NO.: 50:5630c-i,5631a-g
TITLE: Ergot alkaloids. XL. A new synthesis of bufotenine and related hydroxytryptamines
AUTHOR(S): Stoll, A.; Troxler, F.; Peyer, J.; Hofmann, A.
CORPORATE SOURCE: Sandoz, Basel, Switz.
SOURCE: Helvetica Chimica Acta (1955), 38, 1452-72
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 50:27880

AB cf. preceding abstract Nitrosation of m-MeC6H4OH and oxidation of the NO compound give 63% 2,5-(O2N)(HO)C6H3Me, m. 129-30°, which is converted into 87% 2,5-(O2N)(PhCH2O)C6H3Me (I). Treating I mole I with 2 mol (CO2Et)2 and 2 mol EtOK according to Burton and Stoves (C.A. 32, 550.1) at below 8° gives 87% 2-nitro-5-benzyloxyphenylpyruvic acid, m. 112-13°, which (55 g.), reductively cyclized in 600 cc. H2O and 80 cc. 2N NaOH with 70 g. Na2S2O4 added in small portions until the color reaction (deep red) with NaOH is neg. and acidified with dilute HCl, gives 48.5% 5-benzyloxyindole-2-carboxylic acid (II), m. 194-6°. Heating II in quinaldine with Cu powder at 245-50° gives 80% 5-benzyloxyindole (III), m. 103-5°, which, shaken in MeOH with Pd-asbestos (IV) and H, gives 5-hydroxyindole, long needles, m. 107-8°. Treating III in 1:1 EtOH-AcOH with Me2NH and CH2O according to Ek and Witkop (C.A. 49, 12437i) gives 84% 5-benzyloxygramine (V), m. 138°. Adding (20 min.) with stirring 420 cc. MeI to 30 g. V, keeping the mixture 15 h. at 5°, heating the methiodide with 60 g. NaCN in 1.1 l. H2O 2 h. at 80°, extracting the solution with CHCl3, evaporating the CHCl3, taking up the residue (29.6 g.) in 250 cc. Et2O, and diluting the concentrated Et2O solution with petr. ether give 85% 5-benzyloxy-3-indoleacetonitrile (VI), prisms, m. 75-8°. Refluxing 20 g. VI in 140 cc. EtOH and 100 cc. H2O 15 h. with 45 g. KOH, acidifying the mixture with 60 cc. AcOH, and diluting the filtered solution with 500 cc. H2O give 20.6 g. 5-benzyloxy-3-indoleacetic acid, m. 145-7°, which is converted with CH2N2 into the Me ester and the latter heated with N2H4 1.5 h. at 135°, giving 95% 5-benzyloxy-3-indoleacethydrazide (VII), leaflets, m. 153-4°. Adding dropwise 60 cc. N HCl to a mixture of 14.7 g. VII in 250 cc. dioxane and 50 cc. N NaNO2 solution, extracting the acetazide with Et2O, evaporating the Et2O, and treating the residual azide with 50 g. anhydrous Me2NH 3 h. at 5° give 60% 5-benzyloxy-3-indoleacetdimethylamide (VIII), platelets, m. 138-40°. In a similar way the following addnl. amides are prepared: Me, short prisms, m. 141-2°; Et, prisms, m. 126-8°, di-Et, needles, m. 120-1°; H2NCH2CH2, plates, m. 137-9°; and piperidide, leaflets, m. 129-30°. Adding dropwise 1.26 g. LiAlH4 in 200 cc. Et2O in a N atm. to 3.65 g. VIII in 80 cc. THF, stirring the mixture 1 h. at 55°, and working it up in the usual way give 80% 5-benzyloxy-ω-N,N-dimethyltryptamine (bufotenine benzyl ether) (IX), pointed prisms, m. 87-9° [acid oxalate (X), fine leaflets, m. 177-8°]. Similar reduction of the corresponding amides gives the following N-substituted tryptamines: Me, plates, m.

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84-6° [acid oxalate (XI), needles, m. 201-3°]; Et, crystals, m. 59-61° (acid oxalate, short needles, m. 187-9°) [the ω-N,N-diethyl homolog does not crystallize (acid oxalate, prisms, m. 162°)]; H2NCH2CH2, does not crystallize (bis-acid oxalate, leaflets, m. 221-2°); N-[β-(5-benzyloxy-3-indolyl)ethyl]piperidine, prisms, m. 136-8°. Shaking 3.45 g. IX in 75 cc. MeOH with 2 g. 5% IV and H 1.5 h. gives 78% bufotenine (XII), stout prisms, m. 138-40°. With FeCl3 in AcOH and concd. H2SO4, XII gives a reddish color, turning to blue after 1-2 s. The UV absorption curves of XII in EtOH, 0.1N HCl, and 0.1N NaOH, and the IR absorption curves of XII and of natural XII are given. Shaking 1.85 g. X in 200 cc. MeOH with IV in H gives 86% XII acid oxalate, needles, m. 89-90°. Treating 1.1 g. XII in 2 cc. MeOH with 2 cc. MeI 3 h. at 20° gives 1.7 g. XII methiodide, stout prisms, m. 214-15°. Dissolving 2.9 g. XII and 2.3 g. creatinine sulfate (XIII) in 14 cc. N H2SO4 and 40 cc. boiling H2O and dilg. the soln. with Me2CO give a 5.3 g. XII-XIII complex, fine needles, m. 147-9°. Debenzylation of XI gives 5-hydroxy-ω-N-methyltryptamine (ω-N-methylserotonin), short pointed prisms and plates, m. 153-6°; N-Et homolog, short prisms, m. 239-40°; N,N-di-Et homolog, polyhedrons and prisms, m. 147-9° (oxalate, m. 230-2°); N-H2NCH2CH2 analog, bis-acid oxalate, leaflets, m. 208-9°; N-[β-(5-hydroxy-3-indolyl)ethyl]piperidine, stout prisms, m. 201-3° (oxalate, pointed prisms, m. 243-7°). Refluxing 30.6 g. 2,6-O2N(HO)C6H3Me in 150 cc. EtOH contg. 4.6 g. Na 8 h. with 25.4 g. PhCH2Cl, adding H2O, distg. off the EtOH in vacuo, and extg. with Et2O give 63.8% 2,6-O2N(PhCH2O)C6H3Me (XIV), b0.8 170-6°, m. 65-6°. Condensation of XIV with (CO2Et)2 in the presence of EtOK gives the 2-nitro-6-benzyloxyphenylpyruvic acid which is directly converted into 64% (overall) 4-benzyloxy-2-indolecarboxylic acid (XV) (purified via its Na salt), m. 241-2°. Decarboxylation of XV in quinaldine in the presence of Cu powder gives 62% 4-benzyloxyindole (XVI), needles, m. 72-4°, which, treated in MeOH with H in the presence of IV, gives 4-hydroxyindole, hexagonal plates, m. 97-9°. Treating XVI with Me2NH in the same way as in the prepn. of V gives 89% 4-benzyloxygramine (XVII), hexagonal leaflets, m. 94-8°. Treating the methiodide of XVII with NaCN gives 60% 4-benzyloxy-3-indoleacetonitrile, m. 97-100°, which, reduced with LiAlH4, gives 81% 4-benzyloxytryptamine, plates, m. 117-20° [acid oxalate (XVIII), hexagonal plates, m. 188-9°]. Shaking 3.3 g. XVIII in 270 cc. MeOH with Pd and H gives 4-hydroxytryptamine (XIX) oxalate, clusters of platelets, m. 269-70°; free base does not crystallize. XIX-XIII complex, needles, m. 250-5°. Condensation of 121.5 g. 2,4-O2N(PhCH2O)C6H3Me with (CO2Et)2 gives 91% 2-nitro-4-benzyloxyphenylpyruvic acid, m. 133-5° (B. and S. (loc. cit.) found 89-90°), which is converted into 51% 6-benzyloxy-2-indolecarboxylic acid (XX), m. 199-200° (decompn.). Decarboxylation of XX gives 46% 6-benzyloxyindole, leaflets, m. 118-20°, which, with Pd and H in MeOH, gives 6-hydroxyindole (XXI), hexagonal leaflets, m. 124-6°. XXI is converted into 80% 6-benzyloxygramine (XXII), long rods, m. 136-8°. Converting XXII into the methiodide and treating the latter with NaCN give 75% 6-benzyloxy-3-indoleacetonitrile, leaflets, m. 136-7°, which, reduced with LiAlH4 in THF, gives 71% 6-benzyloxytryptamine (XXIII), fine needles, m. 92-6° (oxalate, shiny leaflets, m. 260-5°). XXIII, debenzylated with Pd and H, gives 6-hydroxytryptamine (XXIV) which does not crystallize. XXIII is converted into its sulfate and the latter (1.4 g.) is shaken in 500 cc.

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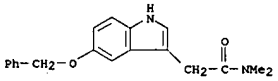
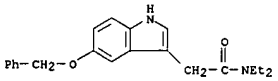
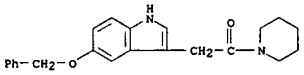
H2O with 500 mg. IV and H, the filtrate concd. to 100 cc., and 0.72 g. XIII added, giving 85% XXIV-XIII complex, fine needles, m. 212-15°. The UV and IR absorption max. of some of the compds. are given.
IT 409111-49-5P, 3-Indoleacetamide, 5-(benzyloxy)-N,N-dimethyl- 857764-35-3P, 3-Indoleacetamide, 5-(benzyloxy)-N,N-diethyl- 872786-56-6P, Piperidine, 1-[[5-(benzyloxy)-3-indolyl]acetyl]- RL: PREP (Preparation)
(preparation of)
RN 409111-49-5 CAPLUS
CN 1H-Indole-3-acetamide, N,N-dimethyl-5-(phenylmethoxy)- (9CI) (CA INDEX NAME)



RN 857764-35-3 CAPLUS
CN 3-Indoleacetamide, 5-(benzyloxy)-N,N-diethyl- (5CI) (CA INDEX NAME)



RN 872786-56-6 CAPLUS
CN Piperidine, 1-[[5-(benzyloxy)-3-indolyl]acetyl]- (5CI) (CA INDEX NAME)



L3 ANSWER 68 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1956:24396 CAPLUS
DOCUMENT NUMBER: 50:24396
ORIGINAL REFERENCE NO.: 50:5035h-i,5036a-d
TITLE: (Hydroxy-3-indolyl)alkylamines
INVENTOR(S): Speeter, Merrill E.
PATENT ASSIGNEE(S): Upjohn Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2708197		19550510	US 1952-289872	19520524

AB (Hydroxy-3-indolyl)alkyl amines are synthesized by the debenzylation of (benzyloxy-3-indolyl)alkylamines (I) prepared by the reduction of (benzyloxy-3-indolyl)alkanoyl amides (II) with Li-AlH4. II are prepared by the Grignard reaction from benzyloxyindole with a haloalkanoyl amide. Thus, a Grignard reagent made from 4.25 g. MeI and 2.4 g. Mg in 200 mL. ether treated with 5.5 g. 5-benzyloxyindole in 200 mL. ether, the mixture refluxed 30 min., cooled in an ice bath, 5.9 g. ClCH2CONMeCH2Ph in 200 mL. ether added, the mixture stirred, the ether distilled off, the residue warmed 3 h. on the steam bath, cooled, 500 mL. ether added, then 5 mL. AcOH in 95 mL. water, and the precipitate allowed to stand overnight and recrystd. from iso-PrOH, yielded 7.5 g. 5-benzyloxy-N-benzyl-N-methyl-3-indoleacetamide (III), m. 151-2°. III (3.84 g.) in 150 mL. THF added with stirring to 3.7 g. LiAlH4 in THF, the mixture refluxed 0.5 h., concentrated to 75 mL., diluted with 500 mL. ether, 50 mL. 5% NaOH added, the ether layer decanted, the water layer reextd. with ether, dilute HCl added to the combined ether layers, and the white precipitate filtered, washed with ether, and recrystd. from EtOH yielded 2.9 g. 5-benzyloxy-3-[2-(benzyl-methylamino)ethyl]indole-HCl (IV), m. 110-12°. A suspension of 2.64 g. IV in 100 mL. H2O treated with 25 mL. 10% NaOH, then 200 mL. ether, the mixture stirred until all the solid dissolved, the ether layer decanted, 3 more extns. with 200-mL. portions of ether made, the exts. washed with H2O, dried over K2CO3, the ether distilled off, the residue dissolved in 25 mL. absolute EtOH, transferred to a microredn. flask, 0.5 g. 10% Pd-C catalyst added, the mixture shaken with H at a little higher than atmospheric pressure at 25° (the H consumption was complete in 0.5 h.), the catalyst filtered off, 13 mL. 0.5N H2SO4 added, the solution concentrated to 5 mL., 1.13 g. creatinine sulfate in 10 mL. H2O added, the resulting pink solution filtered (the rinsings brought the volume to 30 mL.), the solution heated to 60°, 80 mL. acetone added, and the precipitate filtered, dried, and recrystd. from

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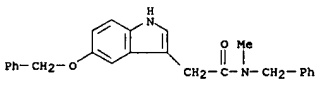
water-acetone yielded 1.3 g. 5-hydroxy-3-(2-methylaminoethyl)indole creatinine sulfate, m. 220-1°. Similarly were synthesized the following 3-substituted-5-hydroxyindole HCl salts (A) and creatinine sulfates (B) (substituent and m.p. given): Me2NCH2CH2 (B), 141-3°; 2-piperidinoethyl (A), 246-8°; Bu2NCH2CH2 (A), 213-14°; also 2-methyl-5-hydroxy-3-(2-aminoethyl)indole-HCl, m. 225.5-7.0°. In similar reactions with ClCH2CN in place of the haloalkanoyl amides were synthesized 5-benzyloxytryptamine-HCl, m. 248-50° (decompn.), and serotonin creatinine sulfate, m. 215-16°. The compds. have potent vasoconstrictor qualities.
IT 725227-53-2P, 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-methyl- RL: PREP (Preparation)
(preparation of)
RN 725227-53-2 CAPLUS
CN 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-methyl- (5CI) (CA INDEX NAME)

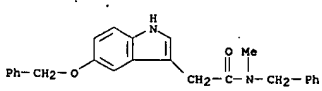


X see 69

L3 ANSWER 69 OF 69 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1955:78071 CAPLUS
DOCUMENT NUMBER: 49:78071
ORIGINAL REFERENCE NO.: 49:14810g-i,14811a
TITLE: (5-Benzyloxy-3-indolyl)alkanamides
INVENTOR(S): Speeter, Merrill E.
PATENT ASSIGNEE(S): Upjohn Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2692882		19541026	US 1952-279931	19520401

GI For diagram(s), see printed CA Issue.
AB I (X is Ph, halophenyl, lower alkoxyphenyl, or lower alkylphenyl; Y is H, Ph, halophenyl, lower alkoxyphenyl, or lower alkylphenyl; R' and R'' are H or lower alkyl; n is 0 or 1; and Z is a secondary amine radical) are prepared by the following exemplary procedure. A Grignard reagent prepared from 4.25 g. MeI and 2.4 g. Mg in 200 ml. Et2O added to 5.5 g. 5-benzyloxyindole in 200 ml. Et2O, the solution refluxed 30 min., cooled in an ice-bath, 5.9 g. ClCH2CONMeCH2Ph in 200 ml. Et2O added, the mixture stirred, the Et2O distilled off, the residue warmed 3 hrs. on a steam bath, cooled, about 500 ml. Et2O added, then, with vigorous stirring, 5 ml. AcOH and 95 ml. H2O, the mixture allowed to stand overnight, and the product filtered and recrystd. gives 7.5 g. 2-(5-benzyloxy-3-indolyl)-N-benzyl-N-methylacetamide, m. 151-2° (from iso-PrOH). Similarly prepared: in 69% yield, the N,N-di-PhCH2 analog, m. 156-7°; and in 30% yield, 2-(5-benzyloxy-3-indolyl)benzylacetamide, m. 185-6°.
IT 725227-53-2P, 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-methyl- 857776-54-6P, 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-isopropyl- 857776-60-4P, 3-Indoleacetamide, N,N-dibenzyl-5-(benzyloxy)- 872786-56-6P, Indole, 5-(benzyloxy)-3-(piperidinocarbonylmethyl)- RL: PREP (Preparation)
(preparation of)
RN 725227-53-2 CAPLUS
CN 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-methyl- (5CI) (CA INDEX NAME)



RN 857776-54-6 CAPLUS
CN 3-Indoleacetamide, N-benzyl-5-(benzyloxy)-N-isopropyl- (5CI) (CA INDEX NAME)

Speeter (892)

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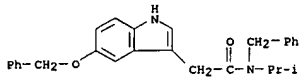
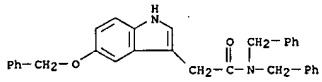


RN 857776-60-4 CAPLUS
CN 3-Indoleacetamide, N,N-dibenzyl-5-(benzyloxy)- (5CI) (CA INDEX NAME)



RN 872786-56-6 CAPLUS
CN Piperidine, 1-[[5-(benzyloxy)-3-indolyl]acetyl]- (5CI) (CA INDEX NAME)